$O(\alpha_s^3 T_F^2 N_f)$ Contributions to the Heavy Flavor Wilson Coefficients of the Structure Function $F_2(x, Q^2)$ at $Q^2 \gg m^2$
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1 Introduction

During the 1950s an intense search for new elementary particles was performed at various particle accelerators which led to the discovery of several hundreds of hadron states. Based on their spin hadrons were classified as mesons (spin = 0, 1) or baryons (spin = 1/2, 3/2). The richness and variety of the hadronic spectrum made it likely, that hadrons are not fundamental particles. First attempts to classify the hadronic spectrum by properties as mass, charge, isospin and flavor were undertaken by W. Heisenberg, M. Gell-Mann and different Japanese groups. In 1961 M. Gell-Mann and Y. Ne’eman independently proposed hadron representations based on the flavor group $SU(3)$, [1–3]. The mesons and spin 1/2-baryon states can be grouped into octets and the spin 3/2-baryon states into decuplets of similar properties. The prediction of the unknown baryon $\Omega^-$ with strangeness $-3$ and electric charge $-1$ was a triumphant success of this theory. A mathematical description of the hadron states was introduced in 1964, when M. Gell-Mann [4], and G. Zweig [5] proposed the static quark-model due to which hadrons are bound states out of three quarks in case of baryons and a quark-antiquark pair for mesons. Here the quarks are assumed to be spin 1/2-fermions. Quantum numbers of all hadron states known by that time could be described assuming three different quark flavors : up ($u$), down ($d$), and strange($s$). The quarks had to carry fractional elementary charges $e_u = +2/3$, $e_d = e_s = -1/3$. The $\Omega^-$–baryon, which is composed out of three $s$-quarks, was obtained as a fermionic state with a spin and flavor–symmetric wave function. Since quarks are fermions, this is not in accordance with the spin-statistics theorem [6–8]. This contradiction was resolved, after some intermediary steps, by introducing the three-valued quantum number color [9–12] for quarks. Since colored particles could not be observed experimentally, it was proposed, that all physical hadron states are color-singlets, [10, 11, 13].

Because of their anomalous magnetic moments, protons and neutrons were suspected to be composite states since the 1930s, cf. [14, 15]. In a series of lepton-nucleon scattering experiments Hofstadter and collaborators [16–19] have shown during the 1950s, that baryons possess extended charge distributions irrespective of their net-charge, which was a further clear sign of compositeness.

In the late 1960s deeply inelastic lepton–nucleon scattering (DIS) experiments at the Stanford Linear Accelerator SLAC, [20, 21], made it possible to study the substructure of nucleons at much higher spatial resolution. One may parametrize the differential scattering cross section in terms of different non–perturbative nucleonic structure functions $F_i$, [22, 23]. They describe the structure of the corresponding hadron at a given energy-transfer $\nu$ in its rest frame and the virtual 4-momentum-transfer from the lepton to the nucleon $q^2 = -Q^2$. The spatial resolution reached is $\Delta x \sim 1/\sqrt{Q^2}$. Based on current algebra techniques J. Bjorken predicted, that in the limit, $Q^2, \nu \to \infty$, $Q^2/\nu = \text{fixed}$, the structure functions do not depend on $Q^2$ and $\nu$ independently but on the Bjorken variable $x = Q^2/2M\nu$, [24]. Here $M$ is the mass of the hadron and $0 < x \leq 1$. This behaviour has been discovered in the SLAC-MIT experiments for nucleons, [25–28] cf. also [29–31]. R. Feynman provided a phenomenological explanation of this behaviour by creating the parton model, [32–34]. The strong correlation between $Q^2$ and $\nu$ in the Bjorken limit can only be understood if the nucleon is composed out of point-like constituents, Feynman’s partons, at short distances. Partons appear as basically massless quantum fluctuations which live long enough to be resolved during the short interaction times $\tau_{\text{int}} \sim 1/g_0$, cf. [35], implying strict conditions for the validity of the parton model.
The hadronic structure functions can then be understood as incoherent weighted sums over individual parton distribution functions \( f_i(x) \) at lowest order. The discovery, that the longitudinal structure function \( F_L \) vanishes in the Bjorken limit, known as Callan-Gross relation [36], showed that the quark-partons possess spin \( 1/2 \). Feynman’s parton model and Gell-Mann’s quark model were finally joint by Bjorken and Paschos [37], who identified the partons as the quarks of the group theoretic approach.

In the 1950s C.N. Yang and R.L. Mills, [38], studied gauge field theories based on non-abelian gauge groups. The non-abelian nature implies three- and quadrilinear couplings between the gauge bosons contrary to the case of Abelian groups, like in Quantum Electrodynamics. The renormalizibility of field theories of this type was proven by G. ’t Hooft [39] in the massless case. In 1972/1973 M. Gell-Mann, H. Fritzsch and H. Leutwyler, [40], cf. also [11], proposed to describe quark interactions by a \( SU(3) \)-Yang-Mills theory. Quantum Chromodynamics (QCD) has been introduced as the dynamical theory of quarks and color–octet vector gluons as gauge bosons. In 1973, D. Gross and F. Wilczek, [41], and H. Politzer, [42], proved that Quantum Chromodynamics is asymptotically free, i.e. the strong coupling decreases toward shorter distances or larger momentum transfer. This allows to perform perturbative computations for scattering processes at large enough momentum scales.

A useful tool to apply perturbative methods in deeply inelastic scattering processes is the light-cone expansion (LCE) [43–46]. Applying it to deeply inelastic scattering processes leads to a factorization theorem, which separates hadronic bound state effects from short distance effects allowing for a perturbative analysis of the operators at the respective twist-level. The long-range bound state effects are collected in the parton distribution functions, which have to be determined from experimental data or computed using non-perturbative methods. The short-distance effects are associated with the Wilson-coefficients and allow for a perturbative analysis.

In 1975 logarithmic scaling violations in the deep inelastic cross section were discovered, [47,48], which are due to the fact that QCD is not a free field theory neither is it conformally invariant, [49]. These scaling violations were predicted perturbatively in higher order calculations and constitute a great success for the Standard Model, [50,51]. Beyond the established light-quark picture a fourth quark, charm, has been proposed [52–54]. It was discovered in 1974 almost simultaneously at SLAC and at Brookhaven National Laboratory (BNL) through the \( J/\psi \) meson. In 1977 the \( \Upsilon \) resonance was observed, [55], which was interpreted as a meson consisting of a new quark, the bottom quark (\( b \)). The search for quarks continued and in 1995 the top quark was discovered at TEVATRON, [56,57].

Today QCD is established as the theory of the strong interaction and together with the electroweak \( SU_L(2) \times U_Y(1) \) sector it forms the Standard Model of elementary particle physics. The electroweak sector of the Standard Model has been introduced by S. Glashow, [58] and S. Weinberg in 1967, [59], cf. also [60,61]. G. ’t Hooft and M. Veltman proved that this theory is renormalizable, [62], see also [63–65].

Deep-inelastic scattering provides a clear method to probe the short distance substructure of hadrons in the space–like domain. Many DIS experiments have been performed through the last forty years, [66–71]. The proton substructure has been examined intensely at HERA at DESY [72–76]. In case of unpolarized deep-inelastic scattering via single photon exchange the cross section is described in terms of the structure functions \( F_2(x,Q^2) \) and \( F_L(x,Q^2) \). While \( F_2 \) has been measured over a wide kinematic range, \( F_L \) has mainly been measured at fixed targets. Experimental data from HERA showed that
the structure functions receive a substantial part due to charm quark pair production, beyond the light flavor contributions which amounts 25–35% in the small \( x \) region, cf. e.g. [77–80].

The scaling violations of the DIS structure functions are determined by the anomalous dimensions and the Wilson coefficients both for the light partons and heavy flavors. The anomalous dimensions have been computed at leading order (LO), [50, 51], and next-to-leading-order (NLO) [81–88]. At next-to-next-to-leading-order (NNLO) fixed moments were obtained in Refs. [89–92] before the general result in the Mellin variable \( N \) was determined in 2004 [93,94] by Vermaseren et al. A first independent check on the NNLO moments of the unpolarized anomalous dimensions was performed in Ref. [95]. The massless Wilson coefficients for the structure functions \( F_2 \) and \( F_L \), resp. their moments, were computed at first order in [96–98], at second order in [99–107], and at third order in [89–92, 108, 109].

Due to the large size of the charm quark contribution to the DIS structure functions the precise computation of these terms is very important. The leading order massive Wilson coefficients have been computed completely in the late 1970s, [110–114]. The NLO–corrections are available in semi-analytic form, [115, 116]. A precise numerical implementation was given in [117]. At three-loop order the computation of the heavy flavor Wilson coefficients over the whole kinematic range appears to be rather difficult at present. However, a very important region for deep-inelastic experiments at HERA can be covered by computing the massive Wilson coefficients for the structure function \( F_2 \) in the limit of \( Q^2 \gg m^2 \). There the heavy flavor Wilson coefficients factorize, cf. Ref. [118], into the process dependent light flavor Wilson coefficients \( C_{(q,g),(2,L)}(x,Q^2/\mu^2) \) and the process independent operator matrix elements (OMEs) \( A_{ij}(x,\mu^2/m^2) \). The OMEs contain all mass dependence and are obtained as matrix elements of the leading twist local composite operators between partonic states \( | j \rangle \) \((i,j = g,q)\). For the structure function \( F_2(x,Q^2) \) this representation becomes effective for \( Q^2 \simeq 10 \) \( m^2 \), cf. [118]. In the case of the longitudinal structure function \( F_L \) this factorization theorem applies for much larger momentum transfers, \( Q^2 \gtrsim 800 \) \( m^2 \), only, [118], which lays outside the kinematic region probed at HERA. The NNLO corrections for the longitudinal structure function have been computed in Ref. [119].

At two-loop order the quarkonic OMEs \( A_{qj} \) have been calculated analytically in Ref. [118] and confirmed, applying rather different methods, in Ref. [120]. The contributions linear in the dimensional parameter \( \varepsilon \) were calculated in Ref. [121]. The remaining gluonic matrix elements \( A_{gj} \) have been derived in Ref. [122]. They were confirmed and extended to \( O(\varepsilon) \) in [123]. The gluonic operator matrix elements are required to describe parton distribution functions in the variable flavor number scheme (VFNS). Furthermore they contribute to the NNLO quarkonic singlet OMEs through renormalization. The complete renormalization procedure for massive 3-loop OMEs was developed in Ref. [95]. There also the general structure of the NNLO OMEs was derived. In Ref. [95] a large amount of Mellin moments for all contributing massive OMEs were computed. All logarithmic terms \( \propto \ln^k(Q^2/m^2) \), \( k = 3, 2, 1 \) are known in full analytic form by now. The mathematical structure of these results is determined by nested harmonic sums [124,125]. Previous analyses of known results of different single–scale hard scattering processes have shown, that at least up to massless three-loop order calculations, single scale results are most simply expressed through nested harmonic sums, [93,94,109,126–130]. They obey algebraic, [131], and structural relations, [132,133]. If one considers fixed moments only,
one obtains representations in terms of multiple zeta values, [134,135].

In the present computation Feynman diagrams are evaluated by direct integration leading to a representation in terms of generalized hypergeometric functions [136,137], cf. also [132]. In the case of massless computations summation algorithms as in Refs. [125, 138,139] can be applied. In the massive case, various additional infinite and finite sums occur which possess a much more involved structure. These sums can be treated applying modern summation technologies encoded in the package *Sigma*, [140–143], written in MATHEMATICA [144].

In Refs. [95, 118–123] all necessary calculations to describe the massive Wilson coefficients in the asymptotic region to 2–loop order and to determine all quantities which have to be known to renormalize these quantities at 3–loop order have been performed. Thereby all logarithmic contributions are known at general values of the Mellin variable \( N \). For an essential piece \(^1\) in the constant part of the renormalized OMEs the general \( N \)–dependence is not known yet. A series of Mellin–moments has been computed in Ref. [95]. The general \( N \) result is of numerical importance and has therefore to be computed exactly. This applies also to its small–\( x \) behaviour which may cause large effects.

In this thesis we perform a first step within this larger programme and compute the \( O(\alpha_s^3T_F^n_f) \) contribution to the massive operator matrix elements \( A_{Qg}, A_{PS}^{PQ}, A_{PS}^{PQ}, A_{NS}^{NS} \) and \( A_{qg,Q}^{TR} \) for general values of the Mellin variable \( N \). Due to the large fraction of the heavy flavor contributions to the deep–inelastic structure functions the precise knowledge of the respective Wilson coefficients is of essential importance to consistently derive the parton distribution functions at leading twist for the gluon, the valence quarks, and for the different sea–quark species, along with a precision measurement of the strong coupling constant \( \alpha_s(M_Z^2) \), cf. e.g. [146]. \( \alpha_s(M_Z^2) \) in itself is one of the fundamental quantities in nature and has to be known as precisely as possible. Note that, despite of a large number of precision analyses using different high–energy observables, a final agreement on the value of \( \alpha_s(M_Z^2) \), being measurable with an accuracy of \( \sim 1\% \) at present, could not be obtained yet, [147]. Needless to say that *all* measurements at the Large Hadron Collider LHC at CERN crucially rely on both the precision knowledge of the parton distribution functions and \( \alpha_s(M_Z^2) \). Furthermore, \( \alpha_s(M_Z^2) \) is an essential input–parameter in scenarios of the potential unification of the fundamental forces of the strong–, weak–, and electromagnetic interactions, cf. [148,149]. Its value is decisive for the question whether, and in which theory, the fundamental forces of nature unify at high energy scales or not. This, in turn, touches the respective scenarios of the physics in the early universe, and is thus also connected to the major challenging problems in physics.

The outline of this thesis is as follows. In Section 2 we describe the basic high–energy process, deeply–inelastic lepton–nucleon scattering, to which the QCD corrections, which are calculated, belong. This includes the QCD-improved parton model at short distances, which is established through the light-cone expansion. The heavy flavor contributions to the deep–inelastic structure functions can be viewed as a linear contribution in addition to the light parton contributions. The leading order corrections in the strong coupling constant are re-calculated in Section 3. We then discuss the general scenario which allows the analytic computation of the heavy flavor corrections to higher orders in the asymptotic region \( Q^2 \gg m^2 \) in terms of massive OMEs and the massless Wilson coefficients. The formalism is outlined to 3–loop orders in Section 4. In Section 5 the details of the renormalization of the massive OMEs are summarized to 3–loop orders. The leading or-

\(^1\)For numerical studies of this aspect see [145].
der massive operator matrix element is then re-calculated in Section 6 as an introductory
calculation, in which we discuss the asymptotic factorization theorem for the heavy flavor
Wilson coefficients following the formalism of Section 4 and compare to the explicit cal-
culation in Section 3. We then turn to the computation of the analytic $O(a_s^{3\alpha_s} T_F^2 N_f C_{F,A})$
contributions to five heavy flavor OMEs at general values of the Mellin variable $N$ in
Section 7. We describe the contributing Feynman diagrams, give details of their analytic
evaluation, and illustrate the methods by different explicit examples. In Section 8 we
present the analytic results for the OMEs $A_{Qg}^{(3)}, A_{Qg}^{PS,(3)}, A_{gq,Q}^{PS,(3)}, A_{qg,Q}^{NS,(3)}$
and $A_{qg,Q}^{NS,TR(3)}$. The new results are the constant parts of the respective unrenormalized 3–loop OMEs and a
first independent recalculation of the corresponding contributions to the 3–loop anom-
lous dimensions. This calculation generalizes results obtained for fixed integer moments in
Ref. [95] to general values of $N$, required by the experimental analyses, for the first time.
The final results are expressed in terms of nested harmonic sums, although intermediary
results require the treatment of generalizations thereof, which finally cancel for the class of
graphs computed. In Section 9 we summarize the main results. A series of technical details
of the present computation is given in the Appendix. Basic conventions are summarized
in Appendix A. A consistent set of Feynman rules for QCD, including those of twist–2
composite operators, is given in Appendix B. Relations for $D$–dimensional momentum
integrals are summarized in Appendix C. In Appendix D the results for the individual
diagrams, which were computed in this thesis, are given for reasons of documentation, to
allow other groups for comparison, and to discuss their mathematical structure. Useful
variable transformations are summarized in Appendix E. The present computation relies
on the use of special higher transcendental functions, which allow a particularly compact
treatment. Main results and relations of these functions, as Euler-integrals, generalized
hypergeometric functions, as well as harmonic sums, are given in Appendix F. The final
results of the present work were obtained summing multiply nested sums of the hyper-
geometric type and their extensions, which are of a sophisticated nature. They could be
uniquely solved using general modern summation technologies encoded in C. Schneider’s
programme package SIGMA [140–143]. As an illustration for several thousands of sums
which had to be computed we show a few examples in Appendix G. Partly they contain a
large amount of also generalized harmonic sums. In Appendix H reference values for the
moments of the 3–loop anomalous dimensions and the various constant parts $a_{ij}^{(3)}$ of the
massive OMEs, being computed in [95], are summarized. These values were used to test
the results of the present calculation.
2 Deeply inelastic scattering

Deep-inelastic scattering (DIS) denotes the scattering process of highly energetic leptons off hadrons, and provides a very precise method to probe the substructure of hadrons at short space-like distances. The 4-momentum transfer $q^2 = -Q^2$ is at least of the order $Q^2 \geq 4\text{GeV}^2$, such that space-like distances of approximately $1/\sqrt{Q^2}$ can be resolved. Different deeply inelastic scattering experiments exploring charged and neutral current reactions allow to probe the flavor and the gluonic structure of the hadron. By performing polarized scattering experiments, also the spin-structure of hadrons can be investigated.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1.png}
\caption{Schematic diagram of deeply inelastic scattering via single boson exchange}
\end{figure}

2.1 Kinematics

The schematic diagram of deep-inelastic scattering at tree level is shown in Figure 1. A lepton with momentum $l$ is scattered off a nucleon with momentum $P$ and mass $M$ via a virtual vector boson. In this process the nucleon state disintegrates and $F$ denotes a new linear combination of hadronic final states with allowed quantum numbers. The momenta of the outgoing lepton and hadronic states are denoted by $l'$ and $P_F$, respectively. The 4-momentum $q$ of the virtual vector boson is space-like and the virtuality $Q^2$ is defined by

$$Q^2 \equiv -q^2 , \quad q = l - l'. \quad (1)$$

Two more independent kinematic variables are sufficient to determine the scattering process:

$$s \equiv (P + l)^2 , \quad (2)$$
$$W^2 \equiv (P + q)^2 = P_F^2 . \quad (3)$$

Here $s$ denotes the total center of momentum energy squared and $W$ is the invariant mass of the final hadron state $\langle P_F \rangle$. The kinematic variables can be measured from the final lepton or hadronic states, depending on the specific experiment, cf. e.g. \cite{150–152}. In the following analysis we will neglect the lepton mass and describe the process using the following Lorentz-invariant kinematic variables:

$$\nu \equiv \frac{P.q}{M} = \frac{W^2 + Q^2 - M^2}{2M} , \quad (4)$$
$$x \equiv \frac{-q^2}{2P.q} = \frac{Q^2}{2M\nu} = \frac{Q^2}{W^2 + Q^2 - M^2} ; \quad (5)$$
$$y \equiv \frac{P.q}{P.l} = \frac{2M\nu}{s - M^2} = \frac{W^2 + Q^2 - M^2}{s - M^2} . \quad (6)$$
Here \( \nu \) is the total energy transfer in the rest frame of the nucleon, \( x \) is a Bjorken variable and \( y \) is the inelasticity, cf. [153]. In general, the momentum \( q \) is transferred via the exchange of a \( \gamma, Z, W^\pm \)–boson. In this thesis we limit the investigation to photon exchange in unpolarized charged lepton-nucleon scattering. For not too large virtualities, i.e. \( Q^2 \leq 500 \) GeV\(^2\), single photon exchange dominates this reaction, cf. [154]. Thus from now on this region will be considered only and weak gauge boson effects caused by the exchange of a \( Z \)-Boson may be disregarded. The invariant hadronic mass obeys the condition

\[
W^2 \geq M^2 .
\]

From (7) one obtains

\[
W^2 = (P + q)^2 = M^2 + Q^2 \left( \frac{1}{x} - 1 \right) \geq M^2 .
\]

Thereby \( x \) is limited to the region

\[
0 \leq x \leq 1 .
\]

For \( x = 1 \) the process is elastic, whereas \( x < 1 \) describes the inelastic region [155]. By considering the nucleon’s rest-frame and demanding a positive energy-transfer, we obtain further restrictions on the kinematic variables:

\[
\nu \geq 0 , \quad 0 \leq y \leq 1 , s \geq M^2 .
\]

The cross section for \( ep \)-scattering is determined by the transition matrix element for the electromagnetic current. In Born approximation it is given by

\[
M_{fi} = e^2 \overline{\upeta}(l', \eta') \gamma^\mu u(l, \eta) \frac{1}{q^2} \langle P_F | J^\mu_{em}(0) | P, \sigma \rangle ,
\]

cf. e.g. [156–158]. Here \( \eta(\eta') \) and \( \sigma \) denote the spin components of the leptons and gluons, respectively. The initial and final hadron states are denoted by \( | P, \sigma \rangle \) and \( \langle P_F | \), respectively. \( \gamma_\mu \) denotes the Dirac-matrices and \( u(\overline{u}) \) are the bi-spinors of the electron and its conjugate, respectively, see Appendix A. Furthermore \( e \) denotes the electric charge and \( J^\mu_{em}(\xi) \) is the quarkonic part of the electromagnetic current operator:

\[
J^\parallel_{\mu}(\xi) = J_{\mu}(\xi) .
\]

For QCD, the electromagnetic current is given by

\[
J^\mu_{em}(\xi) = \sum_{f,f'} \overline{\Psi}_f(\xi) \gamma_\mu \lambda^\mu_{f'f} \Psi_{f'}(\xi) ,
\]

where \( \Psi_f(\xi) \) denotes the quark field of flavor \( f \). \( \lambda^\mu_{f'f} \) describes the electromagnetic charges of the different quark flavors. For three light quark flavors it is given by

\[
\lambda^{em} = \frac{1}{2} \left( \lambda^3_{flavor} + \frac{1}{\sqrt{3}} \lambda^8_{flavor} \right) ,
\]
where the $\lambda^{i}_{\text{flavor}}$ are the Gell-Mann matrices of the flavor group $SU(3)_{\text{flavor}}$, cf. [159,160]. The unpolarized cross section is obtained by averaging over leptonic and hadronic spin degrees of freedom. The differential cross section, cf. [156–158,161], reads:

$$l'_{0}d\sigma/d^{3}l' = \frac{1}{32(2\pi)^{3}}\frac{\alpha^{2}}{(l,P)}\sum_{\eta',\eta,\sigma,F}(2\pi)^{4}\delta^{4}(P_{F} + l' - P - l)|M_{fi}|^{2}.$$  \hfill (15)

Inserting the transition matrix element shows, that the cross section can be decomposed into a tensor $L_{\mu\nu}$ depending only on the leptonic states and a purely hadronic tensor $W_{\mu\nu}$ with

$$L_{\mu\nu}(l,l') = \sum_{\eta',\eta}[\overline{u}_{l'}(\eta')\gamma^{\mu}u(l,\eta)]^{*}[\overline{u}_{l'}(\eta')\gamma^{\nu}u(l,\eta)],$$  \hfill (16)

$$W_{\mu\nu}(q,P) = \frac{1}{4\pi}(2\pi)^{4}\delta^{4}(P_{F} - q - P)(P,\sigma | J^{em}_{\mu}(0) | P_{F} | J^{em}_{\nu}(0) | P,\sigma).$$  \hfill (17)

In terms of these quantities the cross section reads

$$l'_{0}d\sigma/d^{3}l' = \frac{1}{4P.l}\frac{\alpha^{2}}{Q^{4}}L_{\mu\nu}W_{\mu\nu} = \frac{\alpha^{2}}{2(s - M^{2})Q^{4}}L_{\mu\nu}W_{\mu\nu}.$$  \hfill (18)

Here $\alpha$ is the fine structure constant. The leptonic tensor can be computed easily by applying the conventions in Appendix A. One obtains

$$L_{\mu\nu}(l,l') = Tr[/\gamma^{\mu}/\gamma^{\nu}'] = 4\left(l_{\mu}l'_{\nu} + l'_{\mu}l_{\nu} - \frac{Q^{2}}{2}g_{\mu\nu}\right).$$  \hfill (19)

The hadronic tensor cannot be evaluated purely perturbatively due to the non-perturbative nature of the matrix elements\footnote{Ab initio calculations would have to be based on lattice QCD methods. During the last years, an increased numerical precision has been achieved in this field, cf. e.g. [162–167]}. Using the integral representation of the $\delta$-distribution and applying elementary quantum mechanical identities, Eq. (17) can be rewritten as, cf. [158,168],

$$W_{\mu\nu}(q,P) = \frac{1}{4\pi}\sum_{\sigma}\int d^{4}\xi\exp(iq\xi)\langle P | [J^{em}_{\mu}(\xi), J^{em}_{\nu}(0)] | P \rangle$$

$$= \frac{1}{2\pi}\int d^{4}\xi\exp(iq\xi)\langle P | [J^{em}_{\mu}(\xi), J^{em}_{\nu}(0)] | P \rangle.$$  \hfill (20)

Here the bracket $[a,b]$ denotes the commutator of $a$ and $b$. The hadronic tensor obeys various symmetry and conservation laws, cf. [169]. These impose conditions on the Lorentz structure of the hadronic tensor and allow to parametrize it by different scalar structure functions. They contain all information about the structure of the proton. In the general case 14 independent structure functions exist, [170,171], but in the case of unpolarized DIS via single photon exchange only two structure functions contribute. Here the leptonic tensor (16) is symmetric. Since any tensor of rank–2 can be decomposed into a symmetric and an anti-symmetric part, only the symmetric part of the hadronic tensor contributes. Thus the hadronic tensor must be a linear combination of the following tensors

$$g_{\mu\nu}, \ q_{\mu}q_{\nu}, \ P_{\mu}P_{\nu}, \ q_{\mu}P_{\nu} + q_{\nu}P_{\mu}.$$  \hfill (21)
From the conservation of the electromagnetic current,

$$\partial_\mu J^m_\mu(\zeta) = 0 \ ,$$  \hspace{1cm} (22)

Lorentz- and time-reversal invariance it follows that

$$q_\mu W^{\mu\nu} = 0 \ .$$  \hspace{1cm} (23)

Furthermore strong interactions preserve CP-invariance, cf. [172]. Making a general ansatz in terms of (21) and imposing gauge invariance leads to the following representation of $W^{\mu\nu}$, containing the two structure functions $F_L$ and $F_2$

$$W^{\mu\nu}(q, P) = \frac{1}{2x} \left( g_{\mu\nu} + \frac{q_\mu q_\nu}{Q^2} \right) F_L(x, Q^2)$$

$$+ \frac{2x}{Q^2} \left( P_\mu P_\nu + \frac{q_\mu P_\nu + q_\nu P_\mu}{2x} - \frac{Q^2}{4x^2} g_{\mu\nu} \right) F_2(x, Q^2) .$$  \hspace{1cm} (24)

Due to the hermiticity of the hadronic tensor, the structure functions $F_2(x, Q^2)$ and $F_L(x, Q^2)$ are real functions. Their arguments are Bjorken-$x$ and $Q^2$, whereas in the elastic case the cross section is determined by one kinematic variable, e.g. the total energy transfer, only. The differential cross section in terms of the structure function is obtained by inserting (24) into (18):

$$\frac{d\sigma}{dxdy} = \frac{2\pi\alpha^2}{x y Q^2} \left\{ 1 + (1 - y)^2 \left[ F_2(x, Q^2) - y^2 F_L(x, Q^2) \right] \right\} .$$  \hspace{1cm} (25)

The two structure functions $F_2$ and $F_L$ can be extracted from (24) by applying the following projectors in $D$ dimensions:

$$F_L(x, Q^2) = \frac{8x^3}{Q^2} P^\mu P^\nu W^{\mu\nu}(q, P) ,$$

$$F_2(x, Q^2) = \frac{2x}{D - 2} \left[ (D - 1) \frac{4x^2}{Q^2} P^\mu P^\nu W^{\mu\nu}(q, P) - g^{\mu\nu} W^{\mu\nu}(q, P) \right] .$$  \hspace{1cm} (26)

Here and in the following we neglect target mass corrections and thereby set $P^2 = 0$.

### 2.2 The Parton Model

In general, the structure functions in (24) depend on two kinematic variables $Q^2$ and $x$. However, in the Bjorken limit [24] $Q^2, \nu \rightarrow \infty$, $x$ fixed, the structure function depends on $x$ only,

$$\lim_{\{Q^2, \nu\} \rightarrow \infty, \ x = \text{const.}} F_{(2,L)}(x, Q^2) = F_{(2,L)}(x) ,$$  \hspace{1cm} (27)

which is called Bjorken scaling. Experimental observations from electron–proton collisions performed at SLAC in 1968, [25–28], confirmed the existence of an approximate scaling behaviour and thereby supported Bjorken’s predictions. Furthermore it was shown experimentally, that the cross section remained large at high momentum transfers $Q^2$. This
behaviour indicates point-like particles in the target, as no further substructure could be probed with increasing momentum. The earlier picture according to which the size of the proton was about about $10^{-13}$ cm with a smooth charge distribution, \[16,18,19\], which is valid at lower momentum transfer, was superseded. Feynman solved this evanescent contradiction by introducing the parton model, \[32,33\], cf. also \[34,37,156,157,173,174\]. At large enough scales the proton is a composite object, consisting of several point-like particles, the partons. During the interaction time with the virtual photon, the long-lived partons behave as quasi–free particles. The photon scatters elastically of a single parton, while the other partons act as “spectators” and do not interfere with the process. Thus the total cross section is given by the incoherent sum of the individual parton-photon cross sections, weighted by the probability to find a specific parton $i$ with a momentum fraction $z$ inside the proton. Feynman introduced this probability as parton distribution function (PDF), $f_i(z)$. From now on we will use the collinear parton model, according to which the momenta of the specific parton $p$ is taken to be collinear to the nucleon momentum $P$,

$$p = zP . \tag{28}$$

Analogously to the scaling variable $x$ one may define a partonic scaling variable $\tau$,

$$\tau \equiv \frac{Q^2}{2p.q} . \tag{29}$$

Combined with (28) one obtains

$$\tau z = x . \tag{30}$$

Feynman’s original approach, the naive parton model, neglected the radiative corrections. Its main issue consists in the strict correlation

$$\delta \left( \frac{q.p}{M} - \frac{Q^2}{2M} \right) . \tag{31}$$

This condition implies $z = x$. Furthermore, according to this model protons are always composed of two $u$ and one $d$ valence quarks. With the advent of QCD this model was modified and also virtual quark states and gluons were incorporated as additional partons. This more advanced model is known as QCD-improved parton model and can be derived by applying the light-cone expansion. Here the assumption is made, that the hadronic tensor factorizes into the parton distribution functions (PDFs) and a partonic tensor $W_{\mu\nu}^i$:

$$W_{\mu\nu}(x,Q^2) = \frac{1}{4\pi} \sum_i \int_0^1 dz \int_0^1 d\tau \left[ f_i(z) + f_\bar{i}(z) \right] W_{\mu\nu}^i(\tau,Q^2) \delta(x-z\tau) . \tag{32}$$

The partonic tensor is given by (20), where the hadronic states $\langle P |$ are substituted with the corresponding partonic state $\langle p |$ of the struck parton. $f_\bar{i}(z)$ denotes the PDF of the respective anti-parton to parton $i$. Assuming that the electromagnetic parton current takes the following form

$$\langle i | j^i_\mu(\tau) | i \rangle = -ie_i \bar{u}^i \gamma_\mu u^i , \tag{33}$$
where $e_i$ is the charge of the respective parton $i$, one obtains

$$W_{\mu\nu}^i(\tau, Q^2) = \frac{2\pi e_i^2}{q.p} \delta(1 - \tau) \left[ 2p_\mu^i p_\nu^i + p_\mu^i q_\nu + p_\nu^i q_\mu - g_{\mu\nu} q.p i \right].$$

(34)

Combining the $\delta$-distributions in (34) and (32) leads to Feynman’s assumption of the naive parton model: $z = x$. Applying the projectors (26) to the hadronic tensor (32) yields the following structure functions at lowest order:

$$F_L(x, Q^2) = 0,$$

$$F_2(x, Q^2) = x \sum_i e_i^2 \left[ f_i(x) + f_{\bar{i}}(x) \right].$$

(35)

The parton distribution functions are determined from DIS-world data analyses by different groups. Currently they are known to NNLO, i.e. at $O(\alpha_s^3)$, in the unpolarized case, cf. Refs. [146, 175, 176].
3 Calculation of the Wilson coefficients $H_{(2,L),g}^{(1)}$

In the following we calculate the leading order massive Wilson coefficients contributing to the structure functions $F_2(x, Q^2)$ and $F_L(x, Q^2)$ for pure photon exchange. It is given by the Bethe-Heitler fusion process of virtual photon-gluon scattering:

$$\gamma^* + g \to Q + \bar{Q}$$

(36)

![Feynman diagrams](image)

Figure 2: Feynman diagrams contributing to the leading order heavy flavor Wilson coefficient

The Feynman diagrams for the lowest order contributions to this process are shown in Figure 2. The calculation is performed referring to the collinear parton model, i.e. the partons are assumed to act like free particles during the interaction and their momentum is parallel to the proton momentum,

$$k = zP.$$  

(37)

Here $P$ denotes the proton momentum and $k$ is the gluon momentum. The cms velocity $v$ of the outgoing heavy quarks of mass $m$ is then given by

$$v = \left(1 - \frac{m^2}{Q^2} \frac{\tau}{1 - \tau}\right)^{1/2},$$

(38)

where $Q^2$ denotes the negative squared momentum of the space-like photon and $\tau$ is defined as the ratio of the Bjorken-variable $x$ and the momentum fraction $z$,

$$\tau := \frac{x}{z}.$$  

(39)

Applying the Feynman rules, cf. Appendix B, to the diagrams in Figure 2 yields the matrix element

$$M_{\mu\nu} = \bar{u}(p_2)ig_s\gamma_\mu i\frac{p_1 - q + m}{(p_1 - q)^2 - m^2}ie_q\gamma_\nu v(p_1) + \bar{u}(p_2)ig_s\gamma_\mu i\frac{p_1 - k + m}{(p_1 - k)^2 - m^2}ie_q\gamma_\nu v(p_1).$$

(40)

The massive Wilson coefficients are obtained as projections of the squared matrix element

$$H^{\mu\nu\rho\sigma} = M^{\mu\nu}M^{*\rho\sigma}. $$

(41)

Here the sum over the gluon polarization states is performed by contraction with $-g_{\mu\rho}$. The average over the spin directions gives an additional factor of $1/(D-2)$, with $D$ the space-time dimension. The massive Wilson coefficients for $D = 4$ read
\[ H^{(1)}_{2,g} \left( \tau, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) = \frac{T_F}{2} g_{\mu \rho} \int dR_2 \left( g_{\nu \sigma} - 12 \frac{\tau^2}{Q^2} k_\nu k_\sigma \right) H^{\mu \nu \rho \sigma}, \quad (42) \]
\[ H^{(1)}_{L,g} \left( \tau, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) = \frac{T_F}{2} g_{\mu \rho} \int dR_2 \left( -8 \frac{\tau^2}{Q^2} k_\nu k_\sigma \right) H^{\mu \nu \rho \sigma}. \quad (43) \]

Here \( T_F \) is a color factor which is given by \( 1/2 \) for \( SU(N) \), see Appendix A. The phase space integral \( \int dR_2 \) in this case is given by, see e.g. [156],
\[ \int dR_2 = \frac{1}{16 \pi} \frac{1}{\sqrt{s p_{cm}}} \int_0^0 dt, \quad (44) \]
where
\[ p_{cm} = \frac{1}{2 \sqrt{s}} \lambda^{1/2} (s, 0, -Q^2) = \frac{1}{2 \sqrt{s}} \lambda^{1/2} (s, m^2, m^2) \quad (45) \]
denotes the modulus of the center-of-mass 3-momentum of the initial (final) state particles and \( s, t \) the are Mandelstam variables of the \( 2 \to 2 \) process [177], with
\[ \lambda(x, y, z) = (x - y - z)^2 - 4yz. \quad (46) \]
Performing the integration yields :
\[ H^{(1)}_{2,g} \left( \tau, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) = 8 T_F \left\{ v \left[ -\frac{1}{2} + 4 \tau - 4 \tau^2 + 2 \frac{m^2}{Q^2} (\tau^2 - \tau) \right] \right. \]
\[ + \left[ -\frac{1}{2} + \tau - \tau^2 + 2 \frac{m^2}{Q^2} (3 \tau^2 - \tau) + 4 \frac{m^4}{Q^4}, \tau^2 \right] \ln \left( \frac{1 - v}{1 + v} \right) \} \quad (47) \]
\[ H^{(1)}_{L,g} \left( \tau, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) = 16 T_F \left[ v (1 - \tau) + 2 \frac{m^2}{Q^2} \tau^2 \ln \left( \frac{1 - v}{1 + v} \right) \right]. \quad (48) \]
The heavy quark coefficient functions (47) and (48) differ from the results of Ref. [114] by a factor of \( \tau/Q^2 \), which is due to different definitions of the structure functions \( F_2 \) and \( F_L \). In the asymptotic limit \( Q^2 \gg m^2 \) the c.m. velocity \( v \) is written as an expansion in \( (m^2/Q^2) \)
\[ v = 1 - \frac{2m^2}{Q^2} \frac{\tau}{1 - \tau} + O \left( \frac{m^4}{Q^4} \right). \quad (49) \]
In this limit the logarithms in (47) and (48) become
\[ \ln \left( \frac{1 - v}{1 + v} \right) = \ln \left( \frac{m^2}{Q^2} \right) + \ln \left( \frac{\tau}{1 - \tau} \right) + O \left( \frac{m^2}{Q^2} \right). \quad (50) \]
The expansion of (47) and (48) yields

\[ H^{(1)}_{2,g}\left(\tau, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2}\right) = 4T_F \cdot \left\{ 8\tau(1-\tau) - 1 + [\tau^2 + (1-\tau)^2] \ln\left(\frac{Q^2}{m^2}\right) + [\tau^2 + (1-\tau)^2] \ln\left(\frac{1-\tau}{\tau}\right) \right\} + 4T_F \cdot \left\{ -10\tau^2 - \tau + 4(3\tau^2 - \tau) \left[ \ln\left(\frac{\tau}{1-\tau}\right) + \ln\left(\frac{m^2}{Q^2}\right) \right] \right\} + O\left(\frac{m^4}{Q^4}\right), \] (51)

\[ H^{(1)}_{L,g}\left(\tau, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2}\right) = 16T_F \cdot (1-\tau) + 16T_F \cdot \tau^2 \ln\left(\frac{m^2}{Q^2}\right), \] (52)

In the limit \(m^2/Q^2 \to 0\) the Wilson coefficients obtain the following structure:

\[ H^{(1)}_{2,g}\left(\tau, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2}\right) \propto 4T_F \left\{ [\tau^2 + (1-\tau)^2] \ln\left(\frac{Q^2}{m^2}\right) + 8\tau(1-\tau) - 1 \right\}, \] (53)

\[ H^{(1)}_{L,g}\left(\tau, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2}\right) \propto 16T_F \cdot (1-\tau). \] (54)

Often one considers Wilson coefficients in Mellin-space by performing the integral transformation

\[ \tilde{H}_k(N) = \int_0^1 d\tau \tau^{N-1} H(\tau). \] (55)

The factor in front of the logarithm denotes the leading order splitting function [50, 51].

\[ \tilde{P}^{(0)}_{qg}(\tau) = 8T_F[\tau^2 + (1-\tau)^2], \] (56)

which is a process-independent quantity. In Mellin-space it is given by

\[ P^{(0)}_{qg} = 8T_F \frac{N^2 + N + 2}{N(N+1)(N+2)}. \] (57)

The logarithm in (53) indicates the presence of a collinear singularity, if \(m^2 \to 0\). Both (53) and (54) were calculated in the so-called on mass-shell scheme for the outgoing quarks. While (54) is a scheme invariant quantity, redefinitions of the logarithmic contribution in
(53) for $m^2 \to 0$ would yield different expressions, absorbing the divergent term and part of the constant contribution into the gluon distribution. The structure functions $F_{(2, L)}^2$ are obtained by a convolution with the gluon density $G(z, \mu^2)$:

$$
F_{(2, L)}^{Q \bar{Q}}(x, \frac{Q^2}{m^2}) = x \int_{ax}^{1} \frac{dz}{z} H_{(2, L), g} \left( \frac{x}{z}, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) G(z, \mu^2),
$$

where $a = 1 + 4m^2/Q^2$. Inserting (58) into (25) yields the cross section

$$
\frac{d\sigma^{Q \bar{Q}}}{dxdy} = \frac{2\pi\alpha^2}{xyQ^2} \left\{ 1 + (1 - y)^2 \left[ F_2^{Q \bar{Q}}(x, Q^2) - y^2 F_{L}^{Q \bar{Q}}(x, Q^2) \right] \right\}. \tag{59}
$$
4 The Heavy Quark Coefficient Functions in the limit $Q^2 \gg m^2$

We compute the inclusive DIS heavy flavor production cross section in the asymptotic region $Q^2 \gg m^2$. There the heavy flavor Wilson coefficients $H_{i,j}$ and $L_{i,j}$ factorize into massive operator matrix elements $A_{ij}$ and the massless coefficient functions $C_{i,k}$, as has been shown in Ref. [118]. Here $H_{i,j}$ are Wilson coefficients with a photon coupling to the heavy quark line, and $L_{i,j}$ are those with the coupling to a light quark line, see Eqs. (80-84). All process dependent quantities enter only into the light flavor Wilson coefficients, whereas the complete mass dependence is contained in the massive operator matrix elements $A_{ij}$, which are process independent. The power corrections which are proportional to $(m^2/Q^2)^k$, $k \geq 1$, can be disregarded in this limit. A quantitative comparison with the exact LO and NLO result in Refs. [110–114] and [115,116] shows, that in the case of $F_2^{Q\bar{Q}}$ these power corrections can be neglected for $Q^2/m^2 \geq 10$, cf. [118].

Applying the light cone expansion to the partonic tensor corresponding to the inclusive Wilson coefficient $C_{i,j}^{S,PS,NS}$ yields the asymptotic factorization formula, [95]:

$$C_{i,j}^{S,PS,NS,asym}(N, n_f + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}) = \sum_i A_{ij}^{S,PS,NS}(N, n_f + 1, \frac{m^2}{\mu^2}) C_{i,(2,L)}^{S,PS,NS}(N, n_f + 1, \frac{Q^2}{\mu^2}) + O\left(\frac{m^2}{Q^2}\right),$$

(60)

where the quantifier $(n_f + 1)$ denotes one heavy and $n_f$ light flavors and $\mu$ is the factorization scale between the heavy and light contributions in $C_{i,A}$. The light flavor Wilson coefficients are denoted by $C_{i,j}$ and taken at $(n_f + 1)$ flavors. In order to obtain the correct $Q^2$ behaviour, it is necessary to include all radiative corrections containing heavy quark loops into the heavy quark coefficient functions.

Let us consider first the unrenormalized OMEs $\hat{A}_{ij}$. They can be computed as projections of truncated Green’s functions. During the computation of the Green’s functions trace terms emerge. However they do not contribute, since the local operators are traceless. These terms are projected out from the beginning by contracting with

$$J_N \equiv \Delta_{\mu_1}...\Delta_{\mu_N},$$

(61)

where $\Delta_{\mu}$ is a light-like vector. The Green’s functions used for the computation of the OMEs with external gluons are then given by, cf. [118],

$$e^\nu(p)G_{Q,\mu_\nu}^{ab}\epsilon^\nu(p) = e^\nu(p)J_N(\Lambda_{q,a}^\mu(p) | O_{q;\mu_1...\mu_N} | \Lambda_{q,a}^\mu(p))\epsilon^\nu(p),$$

(62)

$$e^\mu(p)G_{q,\mu_\nu}^{ab}\epsilon^\nu(p) = e^\nu(p)J_N(\Lambda_{q,a}^\mu(p) | O_{q;\mu_1...\mu_N} | \Lambda_{q,a}^\mu(p))\epsilon^\nu(p).$$

(63)

Here the external gluon fields are denoted by $\Lambda_{q,a}^\mu$ with color index $a$ and Lorentz index $\mu$. The polarization vectors of the external gluons with momentum $p$ are denoted by $e^\mu(p)$. The indices $q, Q$ of the local operators $O$ label the operator coupled to a light or a heavy quark. In the flavor non-singlet case the following Green’s function contributes

$$\pi(p, s)C_{q,Q}^{ij,NS}\lambda_\nu u(p, s) = J_N(\bar{\Psi}_i(p) | O_{q,\mu_1...\mu_N}^{NS} | \Psi^j(p))_Q.$$  

(64)

Here $u(p, s)$ and $\pi(p, s)$ denote the bi-spinors of the external massless quarks and antiquarks, respectively, and the corresponding fields are $\Psi$ and $\bar{\Psi}$. 

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Further OMEs are obtained from the following Green’s functions with external quarks in the flavor singlet case

\[
\bar{\pi}(p, s)G_Q^{ij}(p, s) = J_N(\bar{\Psi}_i(p) \mid O_{Q,\mu_1...\mu_N} \mid \Psi^j(p)) , \quad (65)
\]

\[
\bar{u}(p, s)G_{q,Q}^{ij}(p, s) = J_N(\bar{\Psi}_i(p) \mid O_{q,\mu_1...\mu_N} \mid \Psi^j(p))Q , \quad (66)
\]

The OMEs \( A_{ij}^{S,PS,NS}(N, n_f + 1) \) are obtained as expectation values of the following twist-2 operators, cf. [178, 179],

\[
O_{q,r;\mu_1...\mu_N}^{NS} = i^{N-1}S[\bar{\psi}\gamma_{\mu_1}D_{\mu_2}...D_{\mu_N}\frac{\lambda_r}{2}\psi] \quad \text{trace terms} , \quad (67)
\]

\[
O_{q,r;\mu_1...\mu_N}^{TR,NS} = \frac{1}{2}i^{N-1}S[\bar{\psi}\sigma_{\mu_1,\mu_2}...D_{\mu_N}\frac{\lambda_r}{2}\psi] \quad \text{trace terms} , \quad (68)
\]

\[
O_{q,r;\mu_1...\mu_N}^{S} = i^{N-1}S[\bar{\psi}\gamma_{\mu_1}D_{\mu_2}...D_{\mu_N}\psi] \quad \text{trace terms} , \quad (69)
\]

\[
O_{q,r;\mu_1...\mu_N}^{S,PS} = 2i^{N-2}SSp[F_a^{\alpha_1\alpha_2}D_{\mu_2}...D_{\mu_{N-1}}F_{\mu_N}^{\alpha_2\alpha_3}] \quad \text{trace terms} , \quad (70)
\]

between corresponding on-shell partonic states \( \langle g \mid O \mid g \rangle \) and \( \sigma^{\mu\nu} = (i/2) [\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu] \). Here \( S \) denotes the symmetrization operator of the Lorentz indices \( \mu_1, ..., \mu_N \), \( D_{\mu} \) is the covariant derivative, \( \Psi \) the quark field and \( F_{\mu\nu} \) is the gluonic field-strength tensor. The flavor matrix of \( SU(n_f) \) is denoted \( \lambda_r \) and \( S \) is the color trace. The operators are classified as flavor singlet (\( S \)) and non-singlet (\( NS \)) with respect to their symmetry properties under the flavor group \( SU(n_f) \).

For \( \hat{A}_{Qg} \) one obtains

\[
\hat{A}_{Qg}(m^2/\mu^2, \varepsilon) = \frac{1}{N_f^2 - 1} \frac{1}{D - 2} (-g_{\mu\nu})\delta_{ab}(-\varepsilon)\delta_{ab}^{(Q,\mu)} . \quad (71)
\]

The OMEs obey the perturbative expansion

\[
A_{ij}^{S,NS}(N, n_f + 1, \frac{m^2}{\mu^2}) = \langle j \mid O_i^{S,NS} \mid j \rangle = \delta_{ij} + \sum_{i=1}^{\infty} a_{ij}^{i,S,NS} . \quad (72)
\]

The singlet contribution has the following representation

\[
A_{qq}^{S} = A_{qq}^{NS} + A_{qq}^{PS} \quad (73)
\]

in terms of the flavor non-singlet (\( NS \)) and the pure-singlet (\( PS \)) contribution.

Since any integral without scale vanishes in dimensional regularization due to the on-shell condition, all corresponding graphs but the \( O(a_0^0) \) term do not contribute. Due to this we have to consider only those matrix elements with at least one heavy mass line. For the singlet terms one has to distinguish the cases in which the operator is inserted on a light or a heavy quark line, respectively a vertex with a number of additional gluon lines, cf. Appendix B. These contributions are referred to as \( A_{qq, Q}^{PS} \) and \( A_{QQ}^{PS} \) in the pure singlet case and by \( A_{qg, Q} \) and \( A_{Qg} \) in the gluonic case. In this thesis we compute contributions to \( A_{qq, Q}^{NS}, A_{qq, Q}^{NS,TR}, A_{PS}^{PS}, A_{qq, Q}^{PS}, \) and \( A_{Qg} \), while the correction to \( A_{Qg} \) will be
given elsewhere [180]. Using the relation

\[ C_{i,(2,L)}^{S,PS,NS} \left( \tau, n_f + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) = C_{i,(2,L)}^{S,PS,NS} \left( \tau, n_f, \frac{Q^2}{\mu^2} \right) \]

\[ + H_{i,(2,L)}^{S,PS} \left( \tau, n_f + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) + L_{i,(2,L)}^{S,PS,NS} \left( \tau, n_f + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) \]

(74)

one may split Eq. (60) into the following contributions, cf. [95],

\[ C_{q,(2,L)}^{PS}(n_f) + L_{q,(2,L)}^{PS}(n_f + 1) = \left[ A_{qq,Q}^{NS}(n_f + 1) + A_{qq,Q}^{PS}(n_f + 1) + A_{Qq}^{PS}(n_f + 1) \right] \]

\[ \times n_f \tilde{C}_{q,(2,L)}^{PS}(n_f + 1) + A_{qq,Q}(n_f + 1) C_{q,(2,L)}^{NS}(n_f + 1) \]

\[ + A_{qg,Q}(n_f + 1)n_f \tilde{C}_{g,(2,L)}^{PS}(n_f + 1) \]

(75)

\[ C_{g,(2,L)}(n_f) + L_{g,(2,L)}(n_f + 1) = A_{gg,Q}(n_f + 1)n_f \tilde{C}_{g,(2,L)}(n_f + 1) \]

\[ + A_{qg,Q}(n_f + 1) C_{q,(2,L)}^{NS}(n_f + 1) \]

\[ + \left[ A_{qg,Q}(n_f + 1) + A_{Qg}(n_f + 1) \right] n_f \tilde{C}_{q,(2,L)}^{PS}(n_f + 1) \]

(76)

\[ H_{q,(2,L)}^{PS}(n_f + 1) = A_{Qq}^{PS}(n_f + 1) \left[ C_{q,(2,L)}^{NS}(n_f + 1) + \tilde{C}_{q,(2,L)}^{PS}(n_f + 1) \right] \]

\[ + \left[ A_{qq,Q}(n_f + 1) + A_{qg,Q}(n_f + 1) \right] \tilde{C}_{q,(2,L)}^{PS}(n_f + 1) \]

\[ + A_{qg,Q}(n_f + 1) \tilde{C}_{g,(2,L)}(n_f + 1) \]

\[ H_{g,(2,L)}(n_f + 1) = A_{gg,Q}(n_f + 1) \tilde{C}_{g,(2,L)}(n_f + 1) + A_{qg,Q}(n_f + 1) \tilde{C}_{q,(2,L)}^{PS}(n_f + 1) \]

\[ + A_{Qg}(n_f + 1) \left[ C_{q,(2,L)}^{NS}(n_f + 1) + \tilde{C}_{q,(2,L)}^{PS}(n_f + 1) \right] \]

(77)

(78)

Here we used the notation

\[ \tilde{f}(n_f) \equiv \frac{f(n_f)}{n_f} \]

(79)

The heavy flavor Wilson coefficients up to \( O(a_s^3) \) can now be obtained by expanding in
Here $\delta_2$ is given by $\delta_2 = 1$ for $F_2$ and by $\delta_2 = 0$ for $F_L$. The relations (80-84) provide the basic scenario for the present work. To 3-loop order they connect the various massive OMEs, $A_{ij}$, and the known massless Wilson coefficients, $C_{(k)}$, to the massive Wilson coefficients in the asymptotic region $Q^2 \gg m^2$. Henceforth, we will calculate the massive operator matrix elements.
5 Renormalization

The renormalization of the massive OMEs proceeds in four steps: i) mass renormalization, ii) renormalization of the strong coupling constant, iii) renormalization of the ultraviolet singularities of the composite local operators, and iv) subtraction of the collinear singularities. To 3-loop order this formalism has been developed in Ref. [95]. In the following we summarize the main steps.

5.1 Renormalization of the Mass

In order to renormalize the heavy quark mass, we will apply the on-shell renormalization scheme and define it as the pole mass. Hence the bare mass \( \hat{m} \) is replaced by

\[
\hat{m} = Z_m m = m \left[ 1 + \hat{a}_s \left( \frac{m^2}{\mu^2} \right)^{\varepsilon/2} \delta m_1 + \hat{a}_s^2 \left( \frac{m^2}{\mu^2} \right)^{\varepsilon} \delta m_2 \right] + O(\hat{a}_s^3) .
\]  

(85)

The constants \( \delta m_1 \) and \( \delta m_2 \) are given by

\[
\delta m_1 = C_F \left[ \frac{6}{\varepsilon} - 4 + \left( 4 + \frac{3}{4} \zeta_2 \right) \varepsilon \right] ,
\]

(86)

\[
\equiv \frac{\delta m_1^{(-1)}}{\varepsilon} + \delta m_1^{(0)} + \delta m_1^{(1)} \varepsilon ,
\]

(87)

\[
\delta m_2 = C_F \left\{ \frac{1}{\varepsilon^2} \left( 18 C_F - 22 C_A + 8 T_F (n_f + N_h) \right) + \frac{1}{\varepsilon} \left( -\frac{45}{2} C_F + \frac{91}{2} C_A \right) 

- 14 T_F (n_f + 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) 

+ T_F \left[ n_f \left( \frac{45}{2} + 10 \zeta_2 \right) + N_h \left( \frac{69}{2} - 14 \zeta_2 \right) \right] \right\}

\]

(88)

\[
\equiv \frac{\delta m_2^{(-2)}}{\varepsilon^2} + \frac{\delta m_2^{(-1)}}{\varepsilon} + \delta m_2^{(0)} .
\]

(89)

Here \( \zeta_k \) is the Riemann \( \zeta \)-function at integer values, cf. (C.10), \( n_f \) denotes the number of light flavors and \( N_h \) the number of heavy flavors, which we will set equal to \( N_h = 1 \) from now on. The pole contributions were given in Refs. [181,182], and the constant term was derived in Refs. [183,184], cf. also [185].

After carrying out mass renormalization up to \( O(\hat{a}_s^3) \) the OMEs have the following
structure
\[ \hat{A}_{ij}(\frac{m^2}{\mu^2}, \varepsilon, N) = \delta_{ij} + \hat{a}_s \hat{A}^{(1)}_{ij}(\frac{m^2}{\mu^2}, \varepsilon, N) + \delta m_1(\frac{m^2}{\mu^2}) \varepsilon^{2} \frac{d}{dm} \hat{A}_{ij}(\frac{m^2}{\mu^2}, \varepsilon, N) \]
\[ + \delta m_2(\frac{m^2}{\mu^2}) \varepsilon^{2} \frac{d}{dm} \hat{A}_{ij}(\frac{m^2}{\mu^2}, \varepsilon, N) + \frac{\delta m_1^2}{2} \left( \frac{m^2}{\mu^2} \right) \varepsilon^{2} \frac{d^2}{dm^2} \hat{A}_{ij}(\frac{m^2}{\mu^2}, \varepsilon, N) \].

\[ (90) \]

Here and in the following we unify all renormalization and factorization scales to one scale \( \mu^2 \).

### 5.2 Renormalization of the Coupling

Considering only \( n_f \) light flavors and no heavy flavors yields the following relation between the bare coupling constant \( \hat{a}_s \) and the renormalized coupling \( a_s^{\overline{MS}} \)
\[ \hat{a}_s = Z_g^{\overline{MS}^2}(\varepsilon, n_f) a_s^{\overline{MS}}(\mu^2) = a_s^{\overline{MS}}(\mu^2) \left[ 1 + \delta a_s^{\overline{MS}}(n_f) a_s^{\overline{MS}}(\mu^2) + \delta a_s^{\overline{MS}^2}(n_f) a_s^{\overline{MS}^2}(\mu^2) \right] + O(a_s^{\overline{MS}^3}) \] .

\[ (91) \]

The coefficients in Eq. (91) are given by [41, 42, 186, 187] and [188, 189],
\[ \delta a_s^{\overline{MS}}(n_f) = \frac{2}{\varepsilon} \beta_0(n_f) , \] \[ \delta a_s^{\overline{MS}^2}(n_f) = \frac{4}{\varepsilon^2} \beta_0^2(n_f) + \frac{1}{\varepsilon} \beta_1(n_f) , \]

with
\[ \beta_0(n_f) = \frac{11}{3} C_A - \frac{4}{3} T_F n_f , \] \[ \beta_1(n_f) = \frac{34}{3} C_A^2 - 4 \left( \frac{5}{3} C_A + C_F \right) T_F n_f . \]

If one considers also heavy flavor contributions it is important to take into account that the factorization condition (60) strictly requires the massless external particles to be on shell. This condition is violated by massive loop insertions to the gluon and ghost-propagators. Fortunately these corrections can be uniquely absorbed into the strong coupling constant, by applying the background field method, cf. [95]. The most direct way to do this, is to perform the renormalization first in the \( \text{MOM} \) scheme and to transform afterwards into the \( \overline{\text{MS}} \) scheme. The following relations are obtained:
\[ a_s^{\text{MOM}} = a_s^{\overline{\text{MS}}} - \beta_0(Q) \ln \left( \frac{m^2}{\mu^2} \right) a_s^{\overline{\text{MS}}^2} \]
\[ + \left[ \beta_0^2(Q) \ln^2 \left( \frac{m^2}{\mu^2} \right) - \beta_1(Q) \ln \left( \frac{m^2}{\mu^2} \right) - \beta_1^{(1)}(Q) \right] a_s^{\overline{\text{MS}}^3} + O(a_s^{\overline{\text{MS}}^4}) \] .

\[ (96) \]
or,

\begin{align}
\bar{a}_s^{\overline{\text{MS}}} &= a_s^{\text{MOM}} + a_s^{\text{MOM}2} \left( \delta a_{s,1}^{\text{MOM}} - \delta a_{s,1}^{\overline{\text{MS}}} (n_f + 1) \right) + a_s^{\text{MOM}3} \left( \delta a_{s,2}^{\text{MOM}} - \delta a_{s,2}^{\overline{\text{MS}}} (n_f + 1) \right) \\
&- 2 \delta a_{s,1}^{\overline{\text{MS}}} (n_f + 1) \left[ \delta a_{s,1}^{\text{MOM}} - \delta a_{s,1}^{\overline{\text{MS}}} (n_f + 1) \right] + O(a_s^{\text{MOM}4}) ,
\end{align}

vice versa, where \( a_s^{\overline{\text{MS}}} = a_s^{\text{MOM}} (n_f + 1) \). These identities are valid to all orders in \( \varepsilon \). In (96) the value for \( \beta_{1,Q} \), [95], are given by

\begin{align}
\beta_{1,Q} &= \hat{\beta}_1(n_f) = -4 \left( \frac{5}{3} C_A + C_F \right) T_F , \\
\beta_{1,Q}^{(1)} &= -\frac{32}{9} T_F C_A + 15 T_F C_F , \\
\beta_{1,Q}^{(2)} &= -\frac{86}{27} T_F C_A - \frac{31}{4} T_F C_F - \zeta_2 \left( \frac{5}{3} T_F C_A + T_F C_F \right) .
\end{align}

5.3 Operator Renormalization and Mass Factorization

The ultraviolet singularities of the composite operators introduced in (67–70) is performed by introducing the corresponding \( Z_{ij} \)-factors:

\begin{align}
O_{q,r;\mu_1,\ldots,\mu_N}^{\text{NS}} &= Z_{q,r;\mu_1,\ldots,\mu_N}^{\text{NS}}(\mu^2) \hat{O}_{q,r;\mu_1,\ldots,\mu_N}^{\text{NS}} , \\
O_{i,j;\mu_1,\ldots,\mu_N}^{\text{PS}} &= Z_{i,j;\mu_1,\ldots,\mu_N}^{\text{PS}}(\mu^2) \hat{O}_{i,j;\mu_1,\ldots,\mu_N}^{\text{PS}} , \quad i = q, g .
\end{align}

Due to their identical quantum numbers mixing occurs among the different singlet operators, (102). The anomalous dimensions of the operators are defined by

\begin{align}
\gamma_{qq}^{\text{NS}} &= \mu Z_{q,q}^{-1,\text{NS}}(\mu^2) \frac{\partial}{\partial \mu} Z_{q,q}^{\text{NS}}(\mu^2) , \\
\gamma_{ij}^{S} &= \mu Z_{il}^{-1,S}(\mu^2) \frac{\partial}{\partial \mu} Z_{ij}^{S}(\mu^2) .
\end{align}

The NS and PS contributions are split in the following way

\begin{align}
Z_{qq}^{-1} &= Z_{qq}^{-1,\text{PS}} + Z_{qq}^{-1,\text{NS}} , \\
A_{qq} &= A_{qq}^{\text{PS}} + A_{qq}^{\text{NS}} .
\end{align}

The anomalous dimensions can be expanded into a perturbative series in \( a_s^{\overline{\text{MS}}} \):

\begin{align}
\gamma_{ij}^{S,\text{PS},\text{NS}}(a_s^{\overline{\text{MS}}}, n_f, N) &= \sum_{l=1}^{\infty} a_s^{\overline{\text{MS}}^l} \gamma_{ij}^{(l),S,\text{PS},\text{NS}}(n_f, N) .
\end{align}

The renormalization is performed in two steps, see [95]. First only \( n_f \) light flavors are considered and then the renormalization scheme is extended to \( n_f \) light and one heavy quark flavor.
In the first case, one finds up to $O(a_s^3)$ up to $O(a_s^{\overline{MS}3})$

$$Z_{ij}(a_s^{\overline{MS}}, n_f) = \delta_{ij} + a_s^{\overline{MS}} \frac{\gamma_{ij}^{(0)}}{\varepsilon} + a_s^{\overline{MS}2} \left\{ \frac{1}{\varepsilon^2} \left( \frac{1}{2} \gamma_{ij}^{(0)} + \beta_0^2 \gamma_{ij}^{(0)} \right) + \frac{1}{2 \varepsilon} \gamma_{ij}^{(1)} \right\}$$

$$+ a_s^{\overline{MS}3} \left\{ \frac{1}{\varepsilon^3} \left( -\frac{1}{6} \gamma_{ij}^{(0)} \gamma_{ij}^{(0)} + \beta_0 \gamma_{ij}^{(0)} + 4 \beta_0^2 \gamma_{ij}^{(0)} \right) \right.$$  

$$+ \frac{1}{\varepsilon^3} \left( \frac{1}{6} \gamma_{ij}^{(1)} \gamma_{ij}^{(0)} + \frac{1}{3} \gamma_{ij}^{(0)} \gamma_{ij}^{(1)} + \frac{2}{3} \beta_0 \gamma_{ij}^{(1)} + 2 \beta_0 \gamma_{ij}^{(0)} + \gamma_{ij}^{(2)} \right) \right\} . \quad (108)$$

As a second step the additional heavy quark is implemented. In order to limit the investigation to the ultraviolet singularities for now, the external momentum is temporarily kept artificially off-shell. The corresponding $Z$-factors for the massive OMEs are then obtained by taking Eq. (108) at $(n_f + 1)$ flavors and applying the scheme transformation (97). Up to $O(a_s^{\text{MOM}3})$ one has

$$Z_{ij}^{-1}(a_s^{\text{MOM}}, n_f + 1, \mu^2) = \delta_{ij} - a_s^{\text{MOM}} \frac{\gamma_{ij}^{(0)}}{\varepsilon} + a_s^{\text{MOM}2} \left[ \frac{1}{\varepsilon} \left( -\frac{1}{2} \gamma_{ij}^{(1)} - \delta a_s^{\text{MOM}1} \gamma_{ij}^{(0)} \right) \right.$$  

$$+ \frac{1}{\varepsilon^2} \left( \frac{1}{2} \gamma_{ij}^{(0)} \gamma_{ij}^{(0)} + \beta_0 \gamma_{ij}^{(0)} \right) \right] + a_s^{\text{MOM}3} \left[ \frac{1}{\varepsilon} \left( -\frac{1}{3} \gamma_{ij}^{(2)} - \delta a_s^{\text{MOM}1} \gamma_{ij}^{(1)} \right) \right.$$  

$$- \delta a_s^{\text{MOM}2} \gamma_{ij}^{(0)} \right) + \frac{1}{\varepsilon^2} \left( \frac{4}{3} \beta_0 \gamma_{ij}^{(1)} + 2 \delta a_s^{\text{MOM}1} \beta_0 \gamma_{ij}^{(0)} + \frac{1}{3} \beta_1 \gamma_{ij}^{(0)} \right) \right.$$  

$$+ \delta a_s^{\text{MOM}1} \gamma_{ij}^{(0)} \gamma_{ij}^{(0)} + \frac{1}{3} \gamma_{ij}^{(0)} \gamma_{ij}^{(1)} + \frac{1}{6} \gamma_{ij}^{(0)} \gamma_{ij}^{(0)} \right] + \frac{1}{\varepsilon^3} \left( -\frac{4}{3} \beta_0^2 \gamma_{ij}^{(0)} \right.$$  

$$- \beta_0 \gamma_{ij}^{(0)} \gamma_{ij}^{(0)} - \frac{1}{6} \gamma_{ij}^{(0)} \gamma_{ij}^{(0)} \right) \right] . \quad (109)$$

The contributions $\propto \delta a_{s,k}^{\text{MOM}}$ in (109) stem from finite mass effects and cancel singularities due to virtual processes at $p^2 \to 0$ in real radiation. The OMEs are split into a purely light part $\hat{A}_{ij}$ and a heavy flavor part $\hat{A}_{ij}^Q$, which denotes any massive OME, we consider:

$$\hat{A}_{ij}(p^2, m^2, \mu^2, a_s^{\text{MOM}}, n_f + 1) = \hat{A}_{ij} \left( \frac{-p^2}{\mu^2}, a_s^{\overline{MS}}, n_f \right)$$

$$+ \hat{A}_{ij}^Q \left( p^2, m^2, \mu^2, a_s^{\text{MOM}}, n_f + 1 \right) . \quad (110)$$

Here the light flavor part $\hat{A}_{ij}$ depends on $a_s^{\overline{MS}}$ since the renormalization prescription for the strong coupling constant applies to the massive part only. The UV–renormalized expression is obtained by subtracting all terms that apply to the light flavors only:

$$\hat{A}_{ij}^Q(p^2, m^2, \mu^2, a_s^{\text{MOM}}, n_f + 1) = Z_{il}^{-1}(a_s^{\text{MOM}}, n_f + 1, \mu^2) \hat{A}_{ij}^Q(p^2, m^2, \mu^2, a_s^{\text{MOM}}, n_f + 1)$$

$$+ Z_{il}^{-1}(a_s^{\text{MOM}}, n_f + 1, \mu^2) \hat{A}_{ij} \left( \frac{-p^2}{\mu^2}, a_s^{\overline{MS}}, n_f \right)$$

$$- Z_{il}^{-1}(a_s^{\overline{MS}}, n_f, \mu^2) \hat{A}_{ij} \left( \frac{-p^2}{\mu^2}, a_s^{\overline{MS}}, n_f \right) . \quad (111)$$
Here $Z_{ij}$ can be expressed as a series in $a_s$ by

$$Z_{ij}^{-1} = \delta_{ij} + \sum_{k=1}^{\infty} a_s^k Z_{ij}^{-1,(k)} . \tag{112}$$

Since in the dimensional regularization scheme all integrals without scale vanish, for the light flavor OMEs only the constant term $\delta_{ij}$ remains in the limit $p^2 \to 0$. Expanding in $a_s$ yields the following UV–finite OME:

$$\bar{A}_{ij}^Q\left(\frac{m^2}{\mu^2}, a_s^{\text{MOM}}, n_f + 1\right) = a_s^{\text{MOM}} \left( \bar{A}_{ij}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(1)}(n_f + 1, \mu^2) - Z_{ij}^{-1,(1)}(n_f) \right)$$

$$+ a_s^{\text{MOM}}^2 \left( \bar{A}_{ij}^{(2),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(2)}(n_f + 1, \mu^2) - Z_{ij}^{-1,(2)}(n_f) \right)$$

$$+ a_s^{\text{MOM}}^3 \left( \bar{A}_{ij}^{(3),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(3)}(n_f + 1, \mu^2) - Z_{ij}^{-1,(3)}(n_f) \right)$$

$$+ Z_{ik}^{-1,(1)}(n_f + 1, \mu^2) \hat{A}_{kj}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) \cdot Z_{ik}^{-1,(2)}(n_f + 1, \mu^2) \hat{A}_{kj}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) . \tag{113}$$

In the on-shell limit $p^2 \to 0$ collinear singularities emerge. These are absorbed into the parton distribution functions and only occur in massless parts of the OMEs. Thus the renormalized OMEs are obtained by

$$A_{ij}^Q\left(\frac{m^2}{\mu^2}, a_s^{\text{MOM}}, n_f + 1\right) = \bar{A}_{il}^Q\left(\frac{m^2}{\mu^2}, a_s^{\text{MOM}}, n_f + 1\right) \Gamma_{lj}^{-1} . \tag{114}$$

The generic renormalization formula is given by

$$A_{ij} = Z_{il}^{-1} \hat{A}_{ik} \Gamma_{kj}^{-1} . \tag{115}$$

In case of massless quarks only the $\Gamma$-factors would be given by, cf. e.g. [118],

$$\Gamma_{ij} = Z_{ij}^{-1} . \tag{116}$$

Due to the fact that collinear singularities emerge in massless subgraphs, only the $\Gamma$-factors have to be computed newly, cf. Ref. [95]. Finally the renormalized operator
matrix element reads:

\[ A^{Q}(\frac{m^{2}}{\mu^{2}}, a_{s}^{MOM}, n_{f} + 1) = \]

\[ a_{s}^{MOM} \left( \hat{A}^{(1),Q}(\frac{m^{2}}{\mu^{2}}) + Z_{ij}^{1,-1}(n_{f} + 1) - Z_{ij}^{1,-1}(n_{f}) \right) \]

\[ + a_{s}^{MOM^{2}} \left( \hat{A}^{(2),Q}(\frac{m^{2}}{\mu^{2}}) + Z_{ij}^{1,-1}(n_{f} + 1) - Z_{ij}^{1,-1}(n_{f}) + Z_{ik}^{1,-1}(n_{f} + 1) \hat{A}^{(1),Q}(\frac{m^{2}}{\mu^{2}}) \right) \]

\[ + \left[ \hat{A}^{(1),Q}(\frac{m^{2}}{\mu^{2}}) + Z_{il}^{1,-1}(n_{f} + 1) - Z_{il}^{1,-1}(n_{f}) \right] \Gamma_{lj}^{1,-1}(n_{f}) \]

\[ + Z_{ik}^{1,-1}(n_{f} + 1) \hat{A}^{(1),Q}(\frac{m^{2}}{\mu^{2}}) + \left[ \hat{A}^{(1),Q}(\frac{m^{2}}{\mu^{2}}) + Z_{il}^{1,-1}(n_{f} + 1) - Z_{il}^{1,-1}(n_{f}) \right] \]

\[ + Z_{ik}^{1,-1}(n_{f} + 1) \hat{A}^{(1),Q}(\frac{m^{2}}{\mu^{2}}) \] \( \Gamma_{lj}^{1,-1}(n_{f}) \) \( + O(a_{s}^{MOM^{4}}) \). \( \text{(117)} \)

One notices that the order \( O(\varepsilon^{2}) \)-terms of the leading order OMEs and the \( O(\varepsilon) \)-terms of the NLO OMEs are required to renormalize the 3–loop OMEs, cf. [118,120–123]. Transforming the coupling constant back into the \( \overline{\text{MS}} \)-scheme and performing a series expansion in \( a_{s}^{\text{MS}} \) yields the final expression for the renormalized OME \( A^{(3)}_{Qg} \), cf. [95],

\[ A^{(3),\overline{\text{MS}}}_{Qg} = \frac{\hat{\gamma}_{gg}^{(0)}}{48} \left\{ (n_{f} + 1)\gamma_{gg}^{(0)} \hat{\gamma}_{gg}^{(0)} + \gamma_{gg}^{(0)} \left( \gamma_{gg}^{(0)} - 2\gamma_{gg}^{(0)} + 6\beta_{0} + 14\beta_{0,Q} \right) + \gamma_{gq}^{(0)} \gamma_{gq}^{(0)} \right\} \]

\[ - 6\beta_{0} - 8\beta_{0,Q} + 8\beta_{0}^{2} + 28\beta_{0,Q} \beta_{0} + 24\beta_{0,Q}^{2} \right\} \ln^{3}(\frac{m^{2}}{\mu^{2}}) + \frac{1}{8} \left\{ \hat{\gamma}_{gg}^{(1)}(\gamma_{gg}^{(0)} - \gamma_{gg}^{(0)}) \right\} \]

\[ - 4\beta_{0} - 6\beta_{0,Q} + 8\gamma_{gg}^{(1)} - \gamma_{gg}^{(1)} + (1 - n_{f})\gamma_{gg}^{(1),PS} + \gamma_{qg}^{(1),NS} + \gamma_{gq}^{(1),NS} - 2\beta_{1} \]

\[ - 2\beta_{1,Q} \right\} \ln^{2}(\frac{m^{2}}{\mu^{2}}) + \frac{\hat{\gamma}_{gg}^{(2)}}{2} - n_{f} \hat{\gamma}_{gg}^{(2)} + \frac{a_{Qg}^{(2)}}{2} \left( \gamma_{gg}^{(0)} - \gamma_{gg}^{(0)} - 4\beta_{0} - 4\beta_{0,Q} \right) \]

\[ + \frac{\hat{\gamma}_{gg}^{(2)}}{2} \left( a_{Qg}^{(2),PS} - n_{f} a_{Qg}^{(2)} \right) + \frac{\hat{\gamma}_{gg}^{(0)} + \hat{\gamma}_{gg}^{(0)}}{16} \left( (n_{f} + 1)\gamma_{gg}^{(0)} + \gamma_{gg}^{(0)} \right) \left( 2\gamma_{gg}^{(0)} - \gamma_{gg}^{(0)} - 6\beta_{0} \right) \]
\begin{align}
-6\beta_{0,Q} & - 4\beta_0[2\beta_0 + 3\beta_{0,Q}] + \gamma_{qq}^{(0)} \left[ -\gamma_{qq}^{(0)} + 6\beta_0 + 4\beta_{0,Q} \right] \right) \ln \left( \frac{m^2}{\mu^2} \right) + \hat{\psi}_{Qg}^{(2)}(\gamma_{gg}^{(0)}) \\
-\gamma_{qq}^{(0)} + 4\beta_0 + 4\beta_{0,Q} & + \hat{\gamma}_{qq}^{(0)} \left( n_f m_{Qq}^{(2),PS} - \overline{m}_{gg,Q}^{(2)} \right) + \frac{\hat{\gamma}_{gg}^{(0)} \zeta_3}{48} \left( (n_f + 1) \gamma_{gg}^{(0)} \gamma_{gg}^{(0)} \right) \\
+ \gamma_{gg}^{(0)} \left[ \gamma_{gg}^{(0)} - 2\gamma_{qq}^{(0)} + 6\beta_0 - 2\beta_{0,Q} \right] + \gamma_{QQ}^{(0)} \left[ \gamma_{QQ}^{(0)} - 6\beta_0 \right] + 8\beta_0^2 - 4\beta_0 \beta_{0,Q} \\
-24\beta_{0,Q}^2 & + \frac{\hat{\gamma}_{gg}^{(1)} \beta_0 \zeta_2}{8} + \frac{\hat{\gamma}_{gg}^{(0)} \zeta_2}{16} \left( \gamma_{gg}^{(1)} - \dot{\gamma}_{gg}^{(1),NS} - \gamma_{QQ}^{(1),NS} - \dot{\gamma}_{qq}^{(1),PS} + 2\beta_1 \right) \\
+ 2\beta_{1,Q} & + \frac{\delta m_1^{(-1)}}{8} \left( 16a_{Qg}^{(2)} + \hat{\gamma}_{gg}^{(0)} \left[ -24\delta m_1^{(0)} - 8\delta m_1^{(1)} - \zeta_2 \beta_0 - 9\zeta_2 \beta_{0,Q} \right] \right) \\
+ \frac{\delta m_1^{(0)}}{2} \left( 2\hat{\gamma}_{gg}^{(1)} - \delta m_1^{(0)} \hat{\gamma}_{gg}^{(0)} \right) + \delta m_1^{(1)} \hat{\gamma}_{gg}^{(0)} \left( \gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} - 2\beta_0 - 4\beta_{0,Q} \right) \\
+ \delta m_2^{(0)} \hat{\gamma}_{gg}^{(0)} + a_{Qg}^{(3)}.
\end{align}

Similar expressions are obtained for the other OMEs, cf. [95]. Both from the unrenormalized and the renormalized OMEs one may extract the information which is new at $O(a_s^3)$:

- the constant parts $a_{ij}^{(3)}(N)$ of the unrenormalized OMEs $\hat{A}_{ij}$

- the corresponding contribution to the 3–loop anomalous dimension $\hat{\gamma}_{ij}^{(2)}(N)$.

Both quantities are computed in the following.
6 Calculation of the Operator Matrix Element $\hat{A}_{Qg}^{(1)}$

As an example to illustrate the method used in principle we recalculate the LO operator matrix element $\hat{A}_{Qg}^{(1)}$ in the following. To the the lowest order in the coupling constant $\hat{a}_s = g_s^2/(4\pi)^2$ it receives contributions from the two Feynman diagrams given in Figure 3. The evaluation of the Feynman amplitudes has been performed using the computer algebra system FORM [190]. One may split off an overall factor

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

from the OMEs, which we will do in the following.

![Feynman diagrams contributing to $\hat{A}_{Qg}^{(1)}$](image)

Figure 3: Feynman diagrams contributing to $\hat{A}_{Qg}^{(1)}$

In the unpolarized case and for pure photon exchange only even moments contribute. This is a consequence of the current crossing relations, cf. e.g. [170,171,191] and the local light cone expansion [43–46]. One obtains

$$\hat{A}_{Qg,(a)}^{(1)} = -8\hat{a}_s T_F S_\epsilon \left( \frac{m^2}{\mu^2} \right)^{\epsilon/2} \frac{1}{(2 + \epsilon)\epsilon} \exp \left( \sum_{l=2}^{\infty} \frac{\zeta_l}{l} \left( \frac{\epsilon}{2} \right)^l \right) \frac{2(N^2 + 3N + 2) + \epsilon(N^2 + N + 2)}{N(N + 1)(N + 2)}$$

$$\hat{A}_{Qg,(b)}^{(1)} = 32\hat{a}_s T_F S_\epsilon \left( \frac{m^2}{\mu^2} \right)^{\epsilon/2} \frac{1}{(2 + \epsilon)\epsilon} \exp \left( \sum_{l=2}^{\infty} \frac{\zeta_l}{l} \left( \frac{\epsilon}{2} \right)^l \right) \frac{1}{(N + 1)(N + 2)}. \quad (120)$$

Here $\hat{a}_s$ denotes the bare coupling constant and $S_\epsilon$ is given by

$$S_\epsilon = \exp \left[ (\gamma_E - \ln(4\pi)) \frac{\epsilon}{2} \right], \quad (122)$$

with

$$\frac{\Gamma(1 - \epsilon/2)}{(4\pi)^{\epsilon/2}} = S_\epsilon \exp \left( \sum_{l=2}^{\infty} \frac{\zeta_l}{l} \left( \frac{\epsilon}{2} \right)^l \right), \quad (123)$$

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cf. Appendix F. One obtains

\[ \tilde{A}_{Qg}^{(1)} = \frac{1}{a_s} \left( \hat{A}_a + \hat{A}_b \right) \]

(124)

\[ = -S_\varepsilon T_F \left( \frac{m^2}{\mu^2} \right)^{\varepsilon/2} \frac{1}{\varepsilon} \exp \left[ -\sum_{l=2}^{\infty} \frac{\zeta_l}{l} \left( \frac{\varepsilon}{2} \right)^l \right] \frac{8(N^2 + N + 2)}{N(N + 1)(N + 2)} \]

(125)

\[ = S_\varepsilon T_F \left( \frac{m^2}{\mu^2} \right)^{\varepsilon/2} \left( -\frac{1}{\varepsilon} - \frac{\zeta_2}{8\varepsilon} - \frac{\zeta_3}{24\varepsilon^2} \right) \frac{8(N^2 + N + 2)}{N(N + 1)(N + 2)} + O(\varepsilon^3) \]

(126)

The \( N \)-dependent term is identified as the Mellin transform of the LO splitting function \( \hat{P}^{(0)}_{qg}(N) \), (56). In \( z \)-space the unrenormalized leading order OME reads

\[ \tilde{A}_{Qg}^{(1)} = S_\varepsilon \left( \frac{m^2}{\mu^2} \right)^{\varepsilon/2} \left[ -\frac{1}{\varepsilon} \hat{P}^{(0)}_{qg}(z) + a^{(1)}_{Qg} + \varepsilon \bar{a}^{(1)}_{Qg} + \varepsilon^2 \bar{a}^{(2)}_{Qg} \right] , \]

(127)

with

\[ a^{(1)}_{Qg} = 0, \]

(128)

\[ \bar{a}^{(1)}_{Qg} = -\frac{\zeta_2}{8} \hat{P}^{(0)}_{qg}(z) \]

(129)

\[ \bar{a}^{(2)}_{Qg} = -\frac{\zeta_3}{24} \hat{P}^{(0)}_{qg}(z) , \]

(130)

cf. Ref. [118]. Expanding up to \( O(\varepsilon^2) \) yields

\[ \tilde{A}_{Qg}^{(1)} = S_\varepsilon \hat{P}^{(0)}_{Qg}(z) \left\{ -\frac{1}{\varepsilon} - \frac{1}{2} \ln \left( \frac{m^2}{\mu^2} \right) - \varepsilon \left[ \ln \left( \frac{1}{8} \frac{m^2}{\mu^2} \right)^2 + \frac{\zeta_2}{8} \right] \\
-\varepsilon^2 \left[ \frac{1}{48} \ln \left( \frac{m^2}{\mu^2} \right)^3 + \frac{\zeta_2}{16} \ln \left( \frac{m^2}{\mu^2} \right) + \frac{\zeta_3}{24} \right] \right\} . \]

(131)

\( \tilde{A}_{Qg}^{(1)} \) possesses a single pole, which is removed by operator renormalization later. The other contributions up to \( O(\varepsilon^2) \) all contribute to the renormalized OME at 3-loop order.

Let us now discuss the results of Section 3, Eqs. (53,54) in the context of the asymptotic heavy flavor Wilson coefficient Eq. (118) to \( O(a_s) \). In case of the structure function \( F_L^{QQ}(x,Q^2) \), \( H^S_{gL} \) is given by the massless result \( \tilde{C}^{(1)}_{gL} \) since \( \delta_2 = 0 \). This applies to all schemes, cf. Ref. [98]. Eq. (54) is actually the same in the heavy and light quark case after performing the limit \( m^2/Q^2 \to 0 \). Comparing \( H_{g2}^{(1)} \), Eq. (53), calculated using the on-mass-shell scheme in Section 3 with the massless result obtained in the \( \overline{\text{MS}} \)-scheme, cf. [98], one obtains the same result. This is in accordance with

\[ a^{(1)}_{Qg} = 0 , \]

(132)

Eq. (132) determining the finite part of \( A_{Qg}^{(1)} \) in Eq. (118). Corrections only occur in \( O(a_s^3) \) and higher. This gives a first illustration of the formalism. The corresponding results at NLO are given in the literature, cf. Refs. [118,120–123].
7 Calculation of the $O(a_s^3 T_F^2 N_f C_F(A))$ Contributions to the Massive Operator Matrix Elements

In the following we describe the computation of the contributions to the massive 3-loop OMEs of $O(T_F^2 n_f C_F A)$ being performed in this thesis. They concern $A_{Qg}$, $A_{PS}^{Qg}$, $A_{qg,Q}^{PS}$, $A_{qg,Q}^{NS}$ in the unpolarized case and $A_{qg,Q}^{NS,TR}$ for transversity. The results for $A_{qg,Q}$ will be presented in [180]. The unrenormalized OMEs are obtained by applying the following projectors to the corresponding truncated Green’s functions. For external gluons the projector $P_g$, cf. [118],

$$P_g \left[ \hat{G}^{ab}_{L,(Q),\mu\nu} \right] \equiv -\frac{\delta_{ab}}{N_c^2 - 1} \frac{g^\mu\nu}{D - 2}(\Delta \cdot p)^{-N} \hat{G}^{ab}_{L,(Q),\mu\nu},$$

(133)
defines the corresponding scalar contributions. In Eq. (133) the summation over $\mu$, $\nu$ includes unphysical gluon-states, which have to be compensated by adding ghost-diagrams. For the external quark contributions the Green’s function is projected by

$$P_q \left[ \hat{G}^{ij}_{L,(Q)} \right] \equiv \frac{\delta^{ij}}{N_c} (\Delta \cdot p)^{-N} \frac{1}{4} \text{Tr}[g^\mu \hat{G}^{ij}_{L,(Q),\mu\nu}].$$

(134)

Another projector is needed for the non-singlet transversity OME. It reads

$$P_{q}^{TR} \left[ \hat{G}^{ij}_{L,(Q)} \right] \equiv -i \frac{\delta^{ij}}{4N_c(D - 2)} (\Delta \cdot p)^{-(N+1)} \left\{ \text{Tr}[\Delta p^\mu \hat{G}^{ij,TR,NS}_{L,(Q),\mu\nu}] - \Delta \cdot p \text{Tr}[p^\mu \hat{G}^{ij,TR,NS}_{L,(Q),\mu\nu}] + i \Delta \cdot p \text{Tr}[\sigma^{\mu\nu} p^\rho \hat{G}^{ij,TR,NS}_{L,(Q),\mu\nu}] \right\},$$

(135)

cf. Ref. [179].

7.1 Contributing diagrams

The Feynman diagrams contributing to the respective Green’s functions have been generated by a code [95, 192] allowing for local operator insertions in QCD-diagrams based on QGRAF, [193]. The diagrams $A_1$ to $R'_1$, see Figure 4, can be generated by including one massless fermion loop into the gluon propagators of the corresponding massive 2-loop diagrams [118,120]. The color factors have been evaluated using the FORM-package color, [194]. For the diagrams that could be obtained from the 2-loop diagrams by inserting a light quark loop, the color factor differs by $T_F n_f$. This massless insertion can easily be integrated out and is given by the following expression for the extended gluon propagator including the quark loop

$$\Pi^{ab}_{\mu\nu}(p_\mu) = \frac{8i g_s^2 T_F n_f}{4\pi^{2+\varepsilon/2}} B \left( 2 + \frac{\varepsilon}{2}, 2 + \frac{\varepsilon}{2} \right) \Gamma \left( -\frac{\varepsilon}{2} \right) \frac{-g_{\mu\nu}p^2 + p_\mu p_\nu}{(p^2)^{2-\varepsilon/2}},$$

(136)

with $g_s$ defined in $D = 4 + \varepsilon$ dimensions.

The main differences to the Feynman rule for the gluon propagator, see Appendix B, are slightly more complicated numerator structures, and the $\varepsilon$ dependence in the power of the denominator. While the new numerator structure in most cases just increased the size
Figure 4: 2-loop diagrams, that were used to generate 3-loop diagrams by the insertion Eq. (136)

Figure 5: Additional ghost diagrams contributing to $A_{Qg}^{(3)}$.
Figure 6: 3-loop diagrams, that are not generated from massive 2-loop graphs

Figure 7: Diagrams contributing to $A_{qq}^{PS}$

Figure 8: Diagrams contributing to $A_{ww,Q}^{PS}$

Figure 9: Diagrams contributing to $A_{ww,Q}^{NS}$
of the computation, the occurrence of real exponents in many cases made it necessary to recompute the decorated 2-loop diagrams completely, since new structures occurred. In Figure 4 we show the 2-loop diagrams of Refs. [118,120] into which the massless fermion-bubble is inserted. This usually concerns more than one line. In some cases the insertions on different gluonic lines lead to different integrals, that cannot be mapped onto each other via a symmetry relation. We labeled this accordingly, e.g. $J_{1b}$, $J_{1b}$, etc. Figures 4 and 5 include the corresponding ghost diagrams which contribute, since the calculation is performed using a $R_\xi$-gauge. In Figure 6 we show the other topologies which contribute to $A_{Qg}$ at $O(T_F^2 n_f C_{F,A})$, but cannot be generated by loop-insertions into known topologies. In this thesis the diagrams $A_2 - H_2$ are computed. In the final result we will show the contributions to $I_2 - L_2$ as well, which are calculated in Ref. [180]. Finally Figures 7–9 show the corresponding diagrams contributing to the OMEs $A_{PS}^{Qg}$, $A_{PS}^{qq,Q}$, and $A_{NS,Q}$, $A_{NS,TR}^{Qg}$. In Tables 1–4 we list the combinatorial multiplicities through which the different diagrams contribute. These were determined from the foregoing computation of the fixed moments for the respective OMEs in [95,192].

Table 1: Multiplicities of the individual diagrams contributing to $A_{Qg}^{(3)}$

| Diagram | Multiplicity | Diagram | Multiplicity | Diagram | Multiplicity |
|---------|--------------|---------|--------------|---------|--------------|
| $A_1$   | 2            | $L_{1a}$ | 4            | $A_2$   | 4            |
| $B_1$   | 4            | $L_{1b}$ | 4            | $B_2$   | 4            |
| $C_1$   | 2            | $M_1$   | 4            | $C_2$   | 2            |
| $D_1$   | 4            | $N_{1a}$ | 4            | $D_2$   | 2            |
| $E_1$   | 4            | $N_{1b}$ | 4            | $E_2$   | 4            |
| $F_1$   | 2            | $O_1$   | 4            | $F_2$   | 8            |
| $G_1$   | 4            | $P_{1a}$ | 2            | $G_2$   | 4            |
| $H_1$   | 2            | $P_{1b}$ | 2            | $H_2$   | 4            |
| $I_1$   | 4            | $S_{1a}$ | 2            | $I_2$   | 4            |
| $J_{1a}$| 2            | $S_{1b}$ | 2            | $J_2$   | 8            |
| $J_{1b}$| 4            | $T_{1a}$ | 1            | $K_2$   | 4            |
| $K_{1a}$| 2            | $T_{1b}$ | 1            | $L_2$   | 8            |
| $K_{1b}$| 4            | $T_{1b}$ | 2            |         |              |

Table 2: Multiplicities of the individual diagrams contributing to $A_{PS}^{Qg}$

| Diagram | Multiplicity |
|---------|--------------|
| $A$     | 4            |
| $B$     | 4            |

3Results on the scalar integrals for diagrams $I_2 - L_2$ are given in Ref. [195] also.
7.2 Evaluation of the Feynman diagrams

The two-loop massive operator matrix elements were calculated in [120, 121, 196]. Prototypes of graphs were computed in [197]. Many diagrams contributing to the $T_{2n_f}$-term of the three loop operator matrix elements can be evaluated by considering the corresponding 2-loop diagrams, see Figure 4, and replacing one gluon propagator by the extended gluon propagator containing the one loop self energy, cf. Figure 10 for an example.

![Figure 10: Replacement of the gluon propagator by an extension including 1-loop massless fermion contributions](image)

The first part of the evaluation of the individual Feynman diagrams has been performed in a procedural way using the algebraic manipulation program FORM, [190]. The occurring fermionic traces of $\gamma$-matrices have been calculated using the built-in functions, before the momenta were integrated. To integrate a respective momentum $k_i$ all denominators containing this variable were combined using Feynman parametrization, see Appendix (C.12). Here the order in which the momenta are integrated is not arbitrary. In many cases specific choices allow to avoid infinite sums emerging from generalized hypergeometric functions. As a next step the $\delta$-distributions are integrated out and the momenta are shifted in order to symmetrize the $D$-dimensional momentum integral. Due to this factors of the form $(\Delta k_i + \Delta l)^N$ occur, where $l$ denotes contributions from other momenta in the form

$$l = P_1(\{x_k\}) k_{j_1} + \cdots + P_n(\{x_n\}) k_{j_n},$$

with polynomials in Feynman parameters $P_i$. These terms have to be expanded using the
binomial theorem prior momentum integration:

\[(\Delta.k_i + \Delta.l)^N = \sum_{j=0}^{N} \binom{N}{j}(\Delta.l)^{N-j}(\Delta.k_i)^j. \quad (138)\]

All but the first terms of this series can be dropped, as the symmetric momentum integrals over odd powers of \(k_i\) vanish and the rules for \(D\)-dimensional integration, cf. Appendix C, lead to terms containing the contraction \(\Delta.\Delta = 0\) for higher powers of \(\Delta.k_i\). In this computation a maximum of the first three terms had to be considered. The symmetric \(D\)-dimensional integral was evaluated by applying the rules in Appendix C. These steps were repeated for all internal momenta, which yields Feynman parameter integrals of various complexity. The application of simple algebraic transformations leads to representations of the following form:

\[I = \sum_{j=0}^{N-2} \int_0^1 \cdots \int_0^1 \prod_{i=1}^n dx_i \frac{(P_1(x_1, \cdots, x_n))^{N-j+n_1}(P_2(x_1, \cdots, x_n))^{j+n_2}}{(1-P(\{x_k\}))^{\frac{3}{2}+n_3}}\]

or

\[I = \int_0^1 \cdots \int_0^1 \prod_{i=1}^n dx_i \frac{(P_1(x_1, \cdots, x_n))^{N+n_4}}{(1-P(\{x_k\}))^{\frac{3}{2}+n_5}}P_3(x_1, \cdots, x_n). \quad (140)\]

Here the \(P_i\) are respective polynomials in the Feynman parameters, \(n_i \in \mathbb{Z}\), and \(P(\{x_k\})\) denotes a product in the Feynman parameters \(\{x_k\}\). The physical sum \(\sum_{j=0}^{N-2}\) emerges if the operator insertion is located at a vertex, cf. Appendix B. In general also diagrams with an operator insertion being represented by a physical double sum \(\sum_{j=0}^{N-3} \sum_{l=j+1}^{N-2}\) have to be computed. For the contributions considered in this paper, these operator insertions where always located on an external vertex. Due to this one of the sums could be performed at the momentum level:

\[\sum_{0 \leq j < l} (\Delta.k - \Delta.p)^{N-l-2}(-\Delta.p + \Delta.q)^{l-j-1}(\Delta.q)^j = \frac{1}{\Delta.p} \sum_{j=0}^{N-2} \left\{ (\Delta.k - \Delta.p)^{N-j-2} \left[ (\Delta.q)^j - (\Delta.q - \Delta.p)^j \right] \right\}, \quad (141)\]

\[\sum_{0 \leq j < l} (\Delta.k - \Delta.p)^{N-l-2}(\Delta.k)^{l-j-1}(\Delta.q)^j = \frac{1}{\Delta.p} \sum_{j=0}^{N-2} \left\{ \left[ (\Delta.k)^j - (\Delta.k - \Delta.p)^j \right] (\Delta.q)^{N-2-j} \right\}. \quad (142)\]

In some cases a simpler structure is obtained, since variable transformations that map that map \(P(\{x_k\})\) to zero are applicable, cf. Appendix E. If possible the physical sums \(\sum_{j=0}^{N-2}\) were evaluated at the Feynman parameter level. All Feynman parameters that could be integrated through substitutions or in terms of Beta-functions were integrated at this point. In case the relations given in Appendix E were not applicable, and no further Feynman parameter could be integrated out directly, the binomial theorem was
used thereby introducing additional finite sums. These steps have been repeated until all Feynman parameters, that do not contribute to the denominator are integrated out. The denominator in (139–140) and remaining Beta-like factors in the Feynman parameters \( \{x_k\} \) were collected in terms of integral representations of generalized hypergeometric functions \( p_{FQ} \), \cite{136,137}. Thus a representation in sums over generalized hypergeometric– and \( \Gamma \)–functions has been obtained. The hypergeometric structure of the Feynman diagram is determined through the mass distribution of the Feynman graph and is widely independent of the operator insertion. We have implemented the relations being listed in Appendix F.2 into a \ FORM \–algorithm, which allowed to perform infinite sums stemming from generalized hypergeometric functions \( p_{FQ} \) on this level in many cases.

The results are now given in terms of finite and infinite sums over \( \Gamma \)–functions depending on the Mellin-variable \( N \) and the dimensional parameter \( \varepsilon \). The respective expressions were simplified and the integrals were expanded into a Laurent series in \( \varepsilon \) using the computer algebra system \ MAPLE \ [198]. In some cases remaining sums could be evaluated by applying known results from the literature, cf. Refs. [120, 121, 199, 200]. More complex sums were evaluated using the \ MATHEMATICA \–based program \ Sigma, [142,143]. Some examples for typical sums that were obtained during this work are given in Appendix G.

For the cases of the diagrams \( A_1–D_1, G_1, J_{1a–K_{1b}} \), the insertion of the massless quark loop changed the structure of the occurring Feynman parameter integrals moderately. The evaluation of these diagrams could be performed in terms of a modification of the computation of the 2-loop results \cite{120}. All other diagrams had to be computed newly.

According to the complexity of the topology, between one and three sums had to be performed after the \( \varepsilon \)-expansion. In the following we demonstrate details of the calculation considering some examples.

### 7.3 Diagram \( E_2 \)

![Diagram E2](image)

Figure 11: The Momentum flow for diagram \( E_2 \)

A typical case for a representation without any remaining sums prior the Laurent expansion is given by diagram \( E_2 \). After applying the projector (133) the color and \( \gamma \)-algebra is performed. The momentum assignment is as follows: \( p_1 = k_1, p_2 = k_1 - k_2, p_3 = k_2, p_4 = k_2 - p, p_5 = k_1 - p, p_6 = k_3, p_7 = k_3 - k_2 \), see Figure 11. One obtains the following representation:

\[
I_{E_2} = T_{\mu}^2 n f C A g_\varepsilon^6 \left( \frac{1}{(\Delta \cdot p)^N} \right) \sum_{j=0}^{N-2} \int \frac{d^D k_1}{(2\pi)^D} \int \frac{d^D k_2}{(2\pi)^D} \int \frac{d^D k_3}{(2\pi)^D} \frac{f(\Delta, k_1, k_2, k_3, p, m, \varepsilon)}{(-k_1^2)(-(k_1 - p)^2)(-k_2^2)(-(k_2 - p)^2)(-(k_1 - k_2)^2)(m^2 - k_3^2)(m^2 - (k_2 - k_3)^2)}^{N-j-2}, \tag{143}
\]

with \( g_\varepsilon \) the strong coupling constant, \( \hat{a}_\varepsilon = g_\varepsilon^2 \cdot (\mu^2)^{\varepsilon/2}/(4\pi)^2 \).
Thus the following representation is obtained

\[ I_{E_2} = T_F^2 n_F C_A g_6 \frac{1}{(\Delta p)^N} \sum_{j=0}^{N-2} \int_0^1 dx_0 \int \frac{d^D k_1}{(2\pi)^D} \int \frac{d^D k_2}{(2\pi)^D} \int \frac{d^D k_3}{(2\pi)^D} \times f(\Delta, k_1, k_2, m, x) \frac{(\Delta, k_3)^j(\Delta, k_3 + \Delta, k_2)^{N-j-2}}{D(k_1, k_2, p, m)(m^2 - k_3^2 - 2x_0k_3k_2 - x_0k_3^2)^2}. \] (144)

Here \( D(k_1, k_2, p, m) \) denotes all the factors in the denominator of (143) which do not depend on the momentum \( k_3 \). In order to symmetrize the momentum integral we shift the momentum \( k_3 \to l_3 - x_0k_2 \). This yields

\[ I_{E_2} = T_F^2 n_F C_A g_6 \frac{1}{(\Delta p)^N} \sum_{j=0}^{N-2} \int_0^1 dx_0 \int \frac{d^D k_1}{(2\pi)^D} \int \frac{d^D k_2}{(2\pi)^D} \int \frac{d^D l_3}{(2\pi)^D} \times f(\Delta, k_1, k_2, m, x, x_1, x_2) \frac{(\Delta, l_3 - x_0\Delta, k_2)^j(\Delta, l_3 + (1 - x_0)\Delta, k_2)^{N-j-2}}{D(k_1, k_2, p, m)(m^2 - k_3^2 - x_0(1 - x_0)k_3^2)^2}. \] (145)

Now we perform a Wick rotation to obtain an Euclidean momentum integral, which can be evaluated as described in Appendix C. The results depend strongly on the momentum structure in the numerator, and become rather lengthy in many cases. During this computation many intermediary results amount to several Mbytes of data. For this reason we consider a numerator of the form

\[ f(\Delta, k_1, k_2, m, N, \varepsilon, x_1, x_2) = m^4 \Delta, p^2 \] (146)

to demonstrate further steps of the computation. In this case only the first term in both powers of the respective binomial expansions of the factors \( (\Delta, l_3 - x_0\Delta, k_2)^j(\Delta, l_3 + (1 - x_0)\Delta, k_2)^{N-j-2} \) contribute. We thereby obtain the following intermediate result after integrating out the momentum \( l_3 \)

\[ I_{E_2} = -T_F^2 n_F C_A g_6 \frac{1}{(\Delta p)^N} \frac{m^4(\Delta, p)^2B(D/2, 2 - D/2)}{(4\pi)^{D/2}\Gamma(-D/2)} \sum_{j=0}^{N-2} (-1)^j x_0^j(1 - x_0)^{N-j-2} \times \int \frac{d^D k_1}{(2\pi)^D} \int \frac{d^D k_2}{(2\pi)^D} \frac{(\Delta, k_2)^{N-2}}{D(k_1, k_2, p, m)(m^2 - x_0(1 - x_0)k_3^2)^2-D/2}. \] (147)

The physical sum can now be evaluated in terms of a geometric sum

\[ \sum_{j=0}^{N-2} (-1)^j x_0^j(1 - x_0)^{N-j-2} = (-1)^N x_0^{N-1} + (1 - x_0)^{N-1}. \] (148)

Thus the following representation is obtained

\[ I_{E_2} = -T_F^2 n_F C_A g_6 \frac{1}{(\Delta p)^N} \frac{m^4(\Delta, p)^2B(D/2, 2 - D/2)}{(4\pi)^{D/2}\Gamma(-D/2)} \times \int_0^1 dx_0 \frac{x_0^{D/2-2}(1 - x_0)^{D/2-2}}{(1 - x_0)^{N-1} + (1 - x_0)^{N-1}} \int \frac{d^D k_1}{(2\pi)^D} \int \frac{d^D k_2}{(2\pi)^D} \times \frac{(\Delta, k_2)^{N-2}}{D(k_2)(-k_1^2)((-k_1 - p)^2)(-k_1 - k_2^2)(m^2/(x_0(1 - x_0)) - k_3^2)^2-D/2}. \] (149)
In the term, which contains the factor $(1 - x_0)^{N-1}$, the variable shift $x_0 \rightarrow (1 - x_0)$ is performed. The same steps as above are applied to integrate over $k_1$. This yields

$$I_{E_2} = -iT_F^2 n_f C_A g_s^6 \frac{m^4 B(D/2, 2 - D/2) B(D/2, 3 - D/2)}{(4\pi)^D \Gamma(-D/2)^2} \int_0^1 dx_0 x_0^{N+D/2-3} (1 - x_0)^{D/2-2} \left(1 + (-1)^N \right)$$

$$\times \int_0^1 dx_2 \int_0^1 dx_3 \theta(1 - x_2 - x_3) \int \frac{d^D k_2}{(2\pi)^D} \left(\Delta, k_2\right)^{N-2}$$

$$\times \frac{D(k_2)(-k_2^2)(-(k_2 - p)^2)(-x_2(1 - x_2)k_2 - x_3 x_3 p)^2(m^2/(x_0(1 - x_0)) - k_2^2)^{2-D/2}}{D(k_2)(-k_2^2)(-(k_2 - p)^2)(-x_2(1 - x_2)k_2 - x_3 x_3 p)^2(m^2/(x_0(1 - x_0)) - k_2^2)^{2-D/2}}.$$  

The transformation $x_3 \rightarrow x_3 (1 - x_2)$ maps the integral restricted by the $\theta$-function to the domain $[0, 1]$. Finally, integrating over the momentum $k_2$, one obtains

$$I_{E_2} = -iT_F^2 n_f C_A g_s^6 \frac{m^4}{(4\pi)^{3/2} \Gamma} \left(8 - \frac{3}{2} D \right)$$

$$\times \int_0^1 dx_0 x_0^{N+D/2-3} (1 - x_0)^{D/2-2} \left[1 + (-1)^N \right]$$

$$\times \int_0^1 dx_2 \int_0^1 dx_3 x_2^{D/2-3} (1 - x_2)^{D/2-2} \int_0^1 dx_7 x_7 (1 - x_7)^{1-D/2}$$

$$\times \int_0^1 dx_5 \int_0^1 dx_6 \theta(1 - x_5 - x_6) x_5^{2-D/2} (1 - x_5 - x_6)^{3-D/2} (x_6 + x_3 x_5)^{N-2}$$

$$\times \left[ \frac{x_0(1 - x_0)}{m^2(1 - x_7)(1 - x_5 - x_6)} \right]^{8-3/2D},$$

with $D = 4 + \varepsilon$. One notices, that after applying the transformation $x_6 \rightarrow (1 - x_5) x_6$ the denominator factorizes into Beta-function like structures. No hypergeometric functions are required to represent this Feynman-integral. The integral over $x_3$ can be directly performed, yielding

$$I_{E_2} = -iT_F^2 n_f C_A g_s^6 \frac{(m^2)^{3/2} \varepsilon}{(4\pi)^{3/2} \Gamma} \left(8 - \frac{3}{2} D \right)$$

$$\times \int_0^1 dx_0 x_0^{5-D+N} (1 - x_0)^{6-D} \left[1 + (-1)^N \right]$$

$$\times \int_0^1 dx_2 x_2^{D/2-3} (1 - x_2)^{D/2-2} \int_0^1 dx_7 x_7 (1 - x_7)^{-7+D}$$

$$\times \int_0^1 dx_5 \int_0^1 dx_6 x_5^{1-D/2} (1 - x_5)^{D-4}(1 - x_6)^{D-5}$$

$$\times \left\{ \frac{1}{N-1} \left[(1 - x_5)^{N-1} x_6^{N-1} - (x_5 + x_6 - x_5 x_6)^{N-1} \right] \right\}.$$  

In the term, which contains the factor $(x_5 + x_6 - x_5 x_6)^{N-1}$, the transformations

$$x_5 \rightarrow x_5 x_6$$

(153)
and

\[ x_6 \to \frac{x_5(1 - x_6)}{1 - x_5x_6}, \]  

(154)

cf. Appendix E, are applied to obtain a representation which can be represented in terms of Beta-functions:

\[
I_{E_2} = T_F^2 n_f C_A g_s^6 \frac{(m^2)^{3/2\varepsilon}}{(4\pi)^{3/2D}} \Gamma \left( \frac{8 - 3}{2} \right) 
\times \int_0^1 dx_0 x_0^{5-D+N} (1 - x_0)^{6-D} \left[ 1 + (-1)^N \right] 
\times \int_0^1 dx_2 x_2^{D/2-3} (1 - x_2)^{D/2-2} \int_0^1 dx_7 x_7(1 - x_7)^{-7+D} 
\times \int_0^1 dx_5 \int_0^1 dx_6 (1 - x_5)^{1-D/2}(x_5)^{D-4}x_6^{D-5} 
\times \frac{1}{N-1} \left[ x_5^{N+5-3/2D}(1 - x_5)^{-6+3/2D}x_6^{6-3/2D} - x_5^{N-1}(1 - x_6)^{N-1} \right]. 
\]  
(155)

Performing the Feynman parameter integrals, and applying the conventions in Appendix A, yields the following representation in terms of \( \Gamma \)-functions:

\[
I_{E_2} = T_F^2 n_f C_A g_s^3 \left( \frac{m^2}{\mu^2} \right)^{3/2\varepsilon} \frac{1}{(4\pi)^{3/2D}} \frac{1}{N-1} \Gamma \left[ \frac{-\varepsilon/2, \varepsilon/2, 1 + \varepsilon/2, \varepsilon - 2, 2 - 3/2\varepsilon, 3 - \varepsilon, 2 + N - \varepsilon}{1 + \varepsilon, 5 + N - 2\varepsilon, N + \varepsilon/2} \right] 
\times \left\{ \Gamma \left[ \frac{N - \varepsilon/2}{1 - \varepsilon/2} \right] - \Gamma(N) \right\} \times \left[ 1 + (-1)^N \right]. 
\]  
(156)

In (156) no more sums remain to be evaluated. Thus, the final result is obtained just by expanding in \( \varepsilon \).

### 7.4 Diagram \( L_{1a} \)

![Figure 12: Momentum flow for diagram \( L_{1a} \)](image)

For this diagram the following representation is obtained after performing the color and Dirac-algebra and integrating out the massless quark insertion:
Here the momentum flow is \( p_1 = k_1, \ p_2 = k_1 - k_2, \ p_3 = k_2, \ p_4 = k_2 - p, \ p_5 = k_1 - p, \) cf. Figure 12. The factor \( (\Delta, k_1)^{N-1} \) in (157) stems from the operator insertion on a quark line. A Feynman-parametrization is applied to combine all the denominators, which contain the momentum \( k_2 \). The emerging \( \delta \)-distribution is integrated out. This yields

\[
I_{L_{1\alpha}} = T_F^2 n_f C_A g_s^6 \Gamma \left[ \frac{-\varepsilon/2, 2 + \varepsilon/2, 2 + \varepsilon/2}{4 + \varepsilon, 1 - \varepsilon/2} \right] \frac{1}{(4\pi)^{D/2}} \frac{1}{(\Delta \cdot p)^N} \int \frac{d^D k_1}{(2\pi)^D} \int \frac{d^D k_2}{(2\pi)^D} \times \frac{f(\Delta \mu, k_1, k_2, p, m, \varepsilon)(\Delta \cdot k_1)^{N-1}}{(-k_2^2)(m^2 - k_2^2)^2((k_2 - k_2)^2 - \epsilon/2)(m^2 - (k_1 - p)^2)(m^2 - (k_1 - k_2)^2)} .
\] (157)

Here \( D(k_1, p, m) \) denotes all the factors in the denominator of (157) that do not depend on the momentum \( k_2 \). In order to symmetrize the momentum integration we shift the momentum \( k_2 \to l_2 + x_1 k_1 + x_2 p \). This yields

\[
I_{L_{1\alpha}} = T_F^2 n_f C_A g_s^6 \Gamma \left[ \frac{-\varepsilon/2, 2 + \varepsilon/2, 2 + \varepsilon/2}{4 + \varepsilon, 1 - \varepsilon/2} \right] \frac{1}{(4\pi)^{D/2}} \frac{1}{(\Delta \cdot p)^N} \int \frac{d^D k_1}{(2\pi)^D} \int \frac{d^D k_2}{(2\pi)^D} \times \frac{f(\Delta \mu, k_1, k_2, p, m, N, \varepsilon)(\Delta \cdot k_1)^{N-1}}{D(k_1, p, m)(-k_2^2 + x_1 m^2 + 2x_1 k_1 k_2 + 2x_2 k_2 p - x_1 k_1^2)^{1-\varepsilon/2}} .
\] (158)

Considering only the contribution

\[
f(\Delta \mu, k_1, l_2, p, m, N, \varepsilon, x_1, x_2) = (\Delta \cdot p) m^4
\] (160)
for now and performing the $l_2$ integral gives

$$I_{L_{1a}} = i T^2_F n_f C_A g_6^2 \frac{1}{(4\pi)^D} \frac{1}{\Delta p^N} \left[ \int \frac{d\Delta k_1}{(2\pi)^D} \right] \frac{\Delta p (\Delta_1)^{N-1}}{(m^2 - k_1^2)(m^2 - (k_1 - p)^2)(m^2 / (1 - x_1) - k_1^2 + 2x_2k_1^2)^{N-1}} \right] \frac{1}{(\Delta p)^N} \left[ \int \frac{d\Delta l_1}{(2\pi)^D} \right] m^4(\Delta_1 + (x_5 + x_2x_6)\Delta p)^{N-1}.$$ 

Combining the remaining denominators inside the momentum integral and symmetrizing by performing the momentum shift $k_1 \rightarrow l_1 + (x_5 + x_2x_6)p$ yields

$$I_{L_{1a}} = i T^2_F n_f C_A g_6^2 \frac{1}{(4\pi)^D} \left[ \int \frac{d\Delta k_1}{(2\pi)^D} \right] \frac{\Delta p (\Delta_1)^{N-1}}{(m^2 - k_1^2)(m^2 - (k_1 - p)^2)(m^2 / (1 - x_1) - k_1^2 + 2x_2k_1^2)^{N-1}} \right] \frac{1}{(\Delta p)^N} \left[ \int \frac{d\Delta l_1}{(2\pi)^D} \right] m^4(\Delta_1 + (x_5 + x_2x_6)\Delta p)^{N-1}.$$ 

When expanding the factor $(\Delta_1 + (x_5 + x_2x_6)\Delta p)^{N-1}$ as described above, only the term $(\Delta p)^{N-3}(x_5 + x_2x_6)^{N-1}$ contributes. Applying the transformation $x_5 \rightarrow x_5(1 - x_6)$ and performing the momentum integration yields

$$I_{L_{1a}} = T^2_F n_f C_A g_6^2 \frac{1}{(4\pi)^{3/2D}} \Gamma \left[ \int \frac{d\Delta k_1}{(2\pi)^D} \right] \frac{\Delta p (\Delta_1)^{N-1}}{(m^2 - k_1^2)(m^2 - (k_1 - p)^2)(m^2 / (1 - x_1) - k_1^2 + 2x_2k_1^2)^{N-1}} \right] \frac{1}{(\Delta p)^N} \left[ \int \frac{d\Delta l_1}{(2\pi)^D} \right] m^4(\Delta_1 + (x_5 + x_2x_6)\Delta p)^{N-1}.$$ 

The factor $(1 - x_5)$ is expanded. For reasons of brevity we will only consider the first
The integral over $x_5$ can be performed directly. Shifting $x_2 \to (1 - x_2)$ gives

$$I_{L_{1a}} = T_F^{2n_f} C g_s^6 \left[ \frac{1}{(4\pi)^{3/2D}} \Gamma \left[ \begin{array}{c} -\varepsilon/2, 2 + \varepsilon/2, 2 + \varepsilon/2, 2 - 3/2\varepsilon \\ 1 - \varepsilon/2, 4 + \varepsilon \end{array} \right] \right]$$

$$\times \int_0^1 dx_1 \int_0^1 dx_2 x_1^{\varepsilon - 1} (1 - x_1)^{2 - \varepsilon} x_2^{-\varepsilon/2}$$

$$\times \int_0^1 dx_6 x_6^{-\varepsilon} (1 - x_6) \frac{1}{(1 - x_1 + x_6 x_1)^{2 - 3/2\varepsilon}}$$

$$\times \frac{1}{N} \left[ (1 - x_6 x_2)^N - (1 - x_2)^N x_6^N \right].$$  \hspace{1cm} (165)

The factor $(1 - x_6 x_2)^N$ cannot simplifed further and a binomial expansion is applied

$$I_{L_{1a}} = T_F^{2n_f} C g_s^6 \left[ \frac{1}{(4\pi)^{3/2D}} \Gamma \left[ \begin{array}{c} -\varepsilon/2, 2 + \varepsilon/2, 2 + \varepsilon/2, 2 - 3/2\varepsilon \\ 1 - \varepsilon/2, 4 + \varepsilon \end{array} \right] \right]$$

$$\times \int_0^1 dx_1 \int_0^1 dx_2 x_1^{\varepsilon - 1} (1 - x_1)^{2 - \varepsilon} x_2^{-\varepsilon/2}$$

$$\times \int_0^1 dx_6 x_6^{-\varepsilon} (1 - x_6) \frac{(\Delta p)^N}{(1 - x_1 + x_6 x_1)^{2 - 3/2\varepsilon}}$$

$$\times \frac{1}{N} \sum_{j_1 = 0}^N (-x_6 x_2)^{j_1} - (1 - x_2)^N x_6^N.$$  \hspace{1cm} (166)

Finally the variable shift $x_6 \to 1 - x_6$ is applied and the integration is performed. We obtain the following result:

$$I_{L_{1a}} = T_F^{2n_f} C A \left( \frac{\mu^2}{\mu^2} \right)^{3/2\varepsilon} \left[ \frac{\delta_s^2}{(4\pi)^{3/2\varepsilon}} \frac{1}{N} \sum_{j_1 = 1}^N \left[ (-1)^{j_1} - \frac{N}{j_1} \delta_{j_1 N} \left( \frac{N}{j_1} \right) \delta_{j_1 N} \right] \right]$$

$$\times \Gamma \left[ \begin{array}{c} -\varepsilon/2, 2 + \varepsilon/2, 2 + \varepsilon/2, 2 - 3/2\varepsilon, 3 - \varepsilon, 1 + j_1 - \varepsilon, 1 + j_1 - \varepsilon/2 \\ 1 - \varepsilon/2, 4 + \varepsilon, 2 + j_1 - \varepsilon/2, 3 + j_1 - \varepsilon \end{array} \right]$$

$$\times {}_3F_2 \left[ \begin{array}{c} 2 - 3/2\varepsilon, 2, \varepsilon \\ 3 + j_1 - \varepsilon, 3 \end{array} ; 1 \right].$$  \hspace{1cm} (167)

As the generalized hypergeometric function in (167) contains both one positive integer in the upper and lower indices, it can be summed by using the relations described in Appendix F.2.

### 7.5 Diagram $I_1$

As a last example we consider diagram $I_1$. It has the following integral representation:

$$I_{I_1} = T_F^{2n_f} g_s^6 \left[ \frac{1}{(\Delta p)^N} \sum_{j=0}^{N-3} \sum_{l=j+1}^{N-2} \int \frac{d^Dk_1}{(2\pi)^D} \int \frac{d^Dk_2}{(2\pi)^D} \int \frac{d^Dk_3}{(2\pi)^D} \right]$$

$$\times \frac{f(\Delta p, k_1, k_2, k_3, p, m, \varepsilon)}{(m^2 - k_1^2) (m^2 - (k_1 - p)^2) (-k_2^2)(m^2 - (k_1 + k_2)^2) (-k_3^2)(-(k_2 - k_3)^2)}. \hspace{1cm} (169)$$
The momentum flow is $p_1 = k_1, p_2 = k_2, p_3 = k_1 + k_2, p_4 = k_1 - p_4$, see Figure 13. One of the sums is performed according to Eqs. (141,142). The integration of the momenta is carried out analogously to earlier examples. Again we limit this demonstration to a small part of the numerator by considering only

$$f(\Delta \mu, k_{1\mu}, k_{2\mu}, k_{3\mu}, p_{\mu}, m, \varepsilon) = (\Delta . p)^3.$$  \hspace{1cm} (170)

Furthermore we limit ourselves to terms which contain the color factor $C_A$. The following representation is obtained:

$$I_{I_1} = T_F^2 n_f C_A a_s^3 \left( \frac{m^2}{\mu^2} \right)^{3/2} \frac{1}{(4\pi)^{3/2} D} \Gamma \left[ \frac{2 + \varepsilon/2, 2 + \varepsilon/2, -3/2\varepsilon}{1 - \varepsilon/2, 4 + \varepsilon} \right] (-1)^N$$

$$\times \int_0^1 dx_0 \int_0^1 dx_1 \int_0^1 dx_1 \int_0^1 dx_3 \sum_{j=0}^{N-2} x_0^j (1 - x_1)^{-1-\varepsilon} (1 - x_1 x_3)^{N-2-j} (1 - x_0 x_1)^{3/2\varepsilon}$$

$$\times \left\{ \left[ (1 - x_1 x_3 (1 - x_0))^j - (x_1 x_3 (1 - x_0))^j \right] \right\}. \hspace{1cm} (171)$$

Here the two terms in the last factor stem from the structure in Eqs. (141-142). Performing the sum $\sum_{j=0}^{N-2}$ in the second term by a geometric sum yields

$$I_{I_1} = T_F^2 n_f C_A a_s^3 \left( \frac{m^2}{\mu^2} \right)^{3/2} \frac{1}{(4\pi)^{3/2} D} \Gamma \left[ \frac{2 + \varepsilon/2, 2 + \varepsilon/2, -3/2\varepsilon}{1 - \varepsilon/2, 4 + \varepsilon} \right] (-1)^N$$

$$\times \int_0^1 dx_0 \int_0^1 dx_1 \int_0^1 dx_1 \int_0^1 dx_3 \sum_{j=0}^{N-2} x_0^j (1 - x_1)^{-1-\varepsilon} (1 - x_1 x_3)^{N-2-j} (1 - x_0 x_1)^{3/2\varepsilon}$$

$$\times \left\{ -(1 - x_1 x_3)^{N-2-j} (x_1 x_3 (1 - x_0))^j$$

$$+ \frac{1}{x_0 x_1 x_3} \left[ (1 - x_1 x_3 (1 - x_0))^{N-1} - (1 - x_1 x_3)^{N-1} \right] \right\}. \hspace{1cm} (172)$$

Due to the stronger nesting of the Feynman parameters, no simplifications by using the variable transformations in Appendix E are possible. The terms $(1 - x_1 x_3 (1 - x_0))^{N-1}$ and $(1 - x_1 x_3)^{N-1}$ are expressed by binomial series. The remaining integral is then evaluated
in terms of the hypergeometric function $3F_2$ yielding the following representation:

$$I_{I_1} = T_F n_f C A a_s^3 \left( \frac{m^2}{\mu^2} \right)^{3/2} \frac{1}{(4\pi)^{3/2} D} \Gamma \left[ \frac{-\varepsilon/2, -3/2 \varepsilon, 2 + \varepsilon/2, 2 + \varepsilon/2, -\varepsilon}{4 + \varepsilon, 1 - \varepsilon/2} \right]$$

$$\left\{ -\sum_{j=0}^{N-2} \sum_{j_1=0}^{N-j-2} \binom{N - j - 2}{j_1} \Gamma \left[ \frac{1 + \varepsilon, 1 + j - \varepsilon, N - j_1 - 1}{2 + j, N - j_1 - \varepsilon} \right] \times 3F_2 \left[ \frac{-3/2 \varepsilon, 1 + \varepsilon, N - j_1}{2 + j, N - j_1 - \varepsilon}; 1 \right] \right.\right.$$ 

$$\left. + \sum_{j_1=0}^{N-1} \binom{N - 1}{j_1} \Gamma \left[ \frac{1 - \varepsilon, \varepsilon, N - j_1 - 1}{N - j_1 - \varepsilon} \right] F_2 \left[ \frac{-3/2 \varepsilon, \varepsilon, N - j_1; 1}{N - j_1 - \varepsilon}; 1 \right] \right.$$ 

$$\left. - \sum_{j_1=0}^{N-1} \binom{N - 1}{j_1} \Gamma \left[ \frac{\varepsilon, N - j_1 - 1}{N - j_1} \right] F_1 \left[ \frac{-3/2 \varepsilon, \varepsilon, N - j_1 - \varepsilon; 1}{N - j_1 - \varepsilon}; 1 \right] \right\}.$$

The Gauss–function $2F_1$ can be mapped to a product of $\Gamma$-functions by applying Gauss' theorem (F.14). Examples for typical sums, emerging after the series expansion in $\varepsilon$ are given in Appendix G.
8 The Massive 3–Loop Operator Matrix Elements and 3–Loop Anomalous Dimensions

In the following we summarize the main results of the calculation. We first obtain the unrenormalized massive operator matrix elements $\hat{A}_{ij}$ for the various channels. Their analytic structure is known, cf. [95]. At 3–loop order two new quantities can be obtained: 

\textit{i) the constant part of the OMEs $A_{ij}^{(3)}$, $a_{ij}^{(3)}$; ii) the three loop anomalous dimension corresponding to the process considered, $\gamma_{ij}^{(2)}$. The latter term is part of the $1/\varepsilon$ pole term of $\hat{A}_{ij}$. We consider the OMEs $A_{Qg}$, $A_{Qq}^{PS}$, $A_{qq,Q}^{NS}$ and $A_{qq,Q}^{NS,TR}$ in the following and determine both quantities. They are represented in terms of the algebraic basis [131] of the harmonic sums, which leads to very essential structural simplifications and avoids redundancies present in other representations for e.g. the 3–loop anomalous dimensions [93, 94] and the massless Wilson coefficients if compared to the representations in [109, 132, 133, 201, 202]. The contributions to the operator matrix elements calculated below constitute the first contributions for general values of $N$ at 3–loop order and, due to Eqs. (80–84), to the heavy flavor Wilson coefficients in the asymptotic region $Q^2 \gg m^2$. The corresponding renormalized OMEs can be obtained following Ref. [95], see also (118), cf. Section 5.

8.1 The gluonic contribution $\hat{A}_{Qg}^{(3)}$

The unrenormalized OME $\hat{A}_{Qg}$ has the following structure, cf. [95],

$$
\hat{A}_{Qg}^{(3)} = \left( \frac{m^2}{\mu^2} \right)^{3\varepsilon/2} \left[ \frac{\gamma_{gg}^{(0)}}{6\varepsilon^3} \left( n_f + 1 \right) \gamma_{gg}^{(0)} \gamma_{gg}^{(0)} + \gamma_{qq}^{(0)} \left[ \gamma_{qq}^{(0)} - 2\gamma_{gg}^{(0)} - 6\beta_0 - 8\beta_{0,Q} \right] + 8\beta_0^2 
+ 28\beta_{0,Q} \beta_0 + 24\beta_0^2 + \gamma_{gg}^{(0)} \left[ \gamma_{gg}^{(0)} + 6\beta_0 + 14\beta_{0,Q} \right] \right) + \frac{1}{6\varepsilon^2} \left[ \gamma_{gg}^{(1)} \left[ 2\gamma_{qq}^{(0)} - 2\gamma_{gg}^{(0)} \right] 
- 8\beta_0 - 10\beta_{0,Q} \right] \right] + \gamma_{gg}^{(0)} \left[ \gamma_{gg}^{(0)} - 3\beta_0 + 5\beta_{0,Q} \right] \right) + \frac{1}{\varepsilon} \left[ \gamma_{gg}^{(2)} - n_f \gamma_{gg}^{(2)} \right] 
+ \gamma_{gg}^{(0)} \left[ a_{gg,Q}^{(2)} - n_f a_{Qg}^{(2,PS)} \right] + a_{Qg}^{(2)} \left[ \gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} - 4\beta_0 - 4\beta_{0,Q} \right] + \frac{\gamma_{gg}^{(0)}}{16} \left[ \gamma_{gg}^{(0)} - 2\gamma_{qq}^{(0)} \right] 
- \gamma_{gg}^{(0)} - 6\beta_0 + 2\beta_{0,Q} \right] \right] \left( n_f + 1 \right) \gamma_{gg}^{(0)} \gamma_{gg}^{(0)} + \gamma_{qq}^{(0)} \left[ -\gamma_{qq}^{(0)} + 6\beta_0 \right] \right] \right] - 8\beta_0^2 
+ 4\beta_{0,Q} \beta_0 + 24\beta_0^2 + \frac{\delta m_1^{(-1)}}{2} \left[ -2\gamma_{gg}^{(1)} + 3\delta m_1^{(-1)} \gamma_{gg}^{(0)} + 2\delta m_1^{(-1)} \gamma_{gg}^{(0)} \right] 
+ \delta m_1^{(0)} \gamma_{gg}^{(0)} \left[ \gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0 + 4\beta_{0,Q} \right] \right] - \delta m_2^{(-1)} \gamma_{gg}^{(0)} \right] + a_{Qg}^{(3)} \right] .
$$

(174)
Here and in the following we always project onto the color factors $T_F^2 n_F C_F$ and $T_F^2 n_F C_A$. The computation performed in this thesis yields:

$$
A_{Qg}^{(3)} = \frac{T_F^2 n_F}{N(N+1)(N+2)} \left\{ C_A \left[ \frac{1}{\varepsilon^3} \left( (N^2 + N + 2) \left( -\frac{512(N^2 + N + 1)}{9(N-1)N(N+1)(N+2)} + \frac{256}{9} S_1 \right) \right] + \frac{1}{\varepsilon^2} \left( (N^2 + N + 2) \left( \frac{128}{9} S_1^2 + \frac{256}{9} S_2 - \frac{128}{9} S_2 S_1 \right) \right) - \frac{128(5N^4 + 20N^3 + 59N^2 + 76N + 20)}{27(N+1)(N+2)} S_1 - \frac{32Q_1(N)}{27(N-1)N^2(N+1)^2(N+2)^2} \right] + \frac{1}{\varepsilon} \left( (N^2 + N + 2) \left( \frac{128}{27} S_1^3 + \frac{32}{3} S_3 \right) + \frac{320}{9} S_2 \right) - \frac{64(N^2 + N + 1)}{3(N-1)N(N+1)(N+2)} \zeta_2 \right) \right) - \frac{128(5N^4 + 14N^3 + 53N^2 + 82N + 20)}{27(N+1)(N+2)} S_2 - \frac{32Q_2(N)}{27(N-1)N(N+1)(N+2)} S_2 \right] \right] + \frac{16Q_4(N)}{81(N-1)N^2(N+1)^3(N+2)^3} \right) \right] + C_F \left[ \frac{1}{\varepsilon^3} \left( (N^2 + N + 2) \left( \frac{64Q_5(N)}{9(N-1)N^2(N+1)^2(N+2)} - \frac{256}{9} S_1 \right) \right] + \frac{1}{\varepsilon^2} \left( (N^2 + N + 2) \left( \frac{128}{27} S_1^2 + \frac{128(5N^3 + 11N^2 + 28N + 12)}{27N} S_1 \right) \right) + \frac{16(N-2)Q_6(N)}{27(N-1)N^3(N+1)^3(N+2)^2} + \frac{1}{\varepsilon} \left( (N^2 + N + 2) \left( -\frac{128}{27} S_1^3 \right) \right) + \frac{704}{27} S_3 - \frac{32}{3} S_3 S_1 - \frac{128}{9} S_2 S_1 + \frac{64(5N^3 + 20N^2 + 37N + 12)}{27N} S_2 \right] + \frac{8(N^2 + N + 2)Q_7(N)}{3(N-1)N^2(N+1)^2(N+2)^2} \zeta_2 + \frac{32Q_7(N)}{9(N-1)N^2(N+1)^2(N+2)} S_2 \right] - \frac{64(10N^4 + 86N^3 + 483N^2 + 341N + 114)}{81N(N+1)} \zeta_2 \right) \right] + \frac{4Q_8(N)}{81(N-1)N^4(N+1)^4(N+2)^3} \right) \right] \right} + a_{Qg}^{(3)} \right) (175)
$$
The contributions due to the individual diagrams are given in (D.2-D.200). The constant part $d_{\nu y}^{(3)}$ reads:

\[
\begin{align*}
\frac{d_{\nu y}^{(3)}}{n_f T_F^2 C_A} & = \left\{ \frac{16(N^2 + N + 2)}{27N(N + 1)(N + 2)} \right\} \left[ 108S_{-2,1,1} - 78S_{2,1,1} - 90S_{-3,1} + 72S_{2,-2} - 6S_{3,1} \\
-108S_{-2,1}S_1 + 42S_{2,1}S_1 - 6S_{-4} + 90S_{-3}S_1 + 118S_3S_1 + 120S_4 + 18S_{-2}S_2 + 54S_{-2}S_1^2 \\
+33S_2S_1^2 + 15S_2^2 + 2S_1^4 + 18S_{-2}\zeta_2 + 9S_2\zeta_2 + 9S_2^2\zeta_2 - 42S_1\zeta_3 \\
+32 \frac{5N^4 + 14N^3 + 53N^2 + 82N + 20}{27N(N + 1)^2(N + 2)^2} [6S_{-2,1} - 5S_{-3} - 6S_{-2}S_1] \\
-64 \frac{5N^4 + 11N^3 + 50N^2 + 85N + 20}{27N(N + 1)^2(N + 2)^2} S_{2,1} \\
-16 \frac{40N^4 + 151N^3 + 544N^2 + 779N + 214}{27N(N + 1)^2(N + 2)^2} S_2 \\
-32 \frac{65N^6 + 429N^5 + 1155N^4 + 725N^3 + 370N^2 + 496N + 648}{81(N - 1)N^2(N + 1)^2(N + 2)^2} S_3 \\
-16 \frac{20N^4 + 107N^3 + 344N^2 + 439N + 134}{81N(N + 1)^2(N + 2)^2} S_1^3 + \frac{Q_9(N)}{81(N - 1)N^3(N + 1)^3(N + 2)^3} S_2 \\
+32 \frac{47N^6 + 278N^5 + 1257N^4 + 2552N^3 + 1794N^2 + 284N + 448}{81N(N + 1)^3(N + 2)^3} S_{-2} \\
+8 \frac{22N^6 + 271N^5 + 6360N^4 + 6816N^3 + 3172N + 1256}{81N(N + 1)^3(N + 2)^3} S_1^2 \\
+ \frac{Q_{10}(N)}{243(N - 1)N^2(N + 1)^4(N + 2)^4} S_1 + \frac{448(N^2 + N + 1)(N^2 + N + 2)}{9(N - 1)N^2(N + 1)^2(N + 2)^2} \zeta_3 \\
-16 \frac{5N^4 + 20N^3 + 59N^2 + 76N + 20}{9N(N + 1)^2(N + 2)^2} S_1\zeta_2 - \frac{Q_{11}(N)}{9(N - 1)N^3(N + 1)^3(N + 2)^3} \zeta_3 \\
-\frac{Q_{12}(N)}{243(N - 1)N^5(N + 1)^5(N + 2)^5} \right\} \right. \\
+ n_f T_F^2 C_F \left\{ \frac{16(N^2 + N + 2)}{27N(N + 1)(N + 2)} \right\} \left[ 144S_{2,1,1} - 72S_{3,1} - 72S_{2,1}S_1 + 48S_4 + 16S_3S_1 \\
-24S_2^2 - 12S_2S_1^2 - 2S_1^4 - 9S_1^2\zeta_2 + 42S_1\zeta_3 \\
+32 \frac{10N^3 + 49N^2 + 83N + 24}{81N^2(N + 1)(N + 2)} [3S_2S_1 + S_1^3] \\
-128(N^2 - 3N - 2)S_{2,1} - \frac{Q_{13}(N)}{81(N - 1)N^3(N + 1)^3(N + 2)^2} S_3 \\
+ \frac{Q_{14}(N)}{27(N - 1)N^4(N + 1)^4(N + 2)^3} S_2 = \frac{32(10N^4 + 185N^3 + 789N^2 + 521N + 141)}{81N^2(N + 1)^2(N + 2)} S_1^2 \\
-16 \frac{230N^5 - 924N^4 - 5165N^3 - 7454N^2 - 10217N - 2670}{243N^2(N + 1)^3(N + 2)^3} S_1 \\
+16 \frac{5N^3 + 11N^2 + 28N + 12}{9N^2(N + 1)(N + 2)} S_1\zeta_2 - \frac{Q_{15}(N)}{9(N - 1)N^3(N + 1)^3(N + 2)^2} \zeta_3 \\
+ \frac{Q_{16}(N)}{9(N - 1)N^4(N + 1)^4(N + 2)^3} \zeta_3 + \frac{Q_{17}(N)}{243(N - 1)N^6(N + 1)^6(N + 2)^5} \right\} ,
\end{align*}
\]
with the polynomials

\[ Q_1(N) = 15N^9 + 90N^8 + 146N^7 - 32N^6 - 501N^5 - 610N^4 - 244N^3 - 48N^2 + 224N + 96, \]  
\[ Q_2(N) = 10N^6 + 105N^5 + 231N^4 + 109N^3 + 143N^2 + 122N + 144, \]  
\[ Q_3(N) = 11N^6 + 32N^5 + 363N^4 + 848N^3 + 186N^2 - 520N + 88, \]  
\[ Q_4(N) = 273N^{12} + 2565N^{11} + 9838N^{10} + 18902N^9 + 14303N^8 - 8953N^7 - 26402N^6 - 19930N^5 - 1860N^4 + 4512N^3 - 2560N^2 - 2208N - 576, \]  
\[ Q_5(N) = 3N^6 + 9N^5 - N^4 - 17N^3 - 38N^2 - 28N - 24, \]  
\[ Q_6(N) = 45N^{10} + 405N^9 + 1606N^8 + 3842N^7 + 6717N^6 + 9325N^5 + 10888N^4 + 9804N^3 + 6232N^2 + 3264N + 864, \]  
\[ Q_7(N) = 3N^8 + 62N^7 + 150N^6 - 8N^5 - 357N^4 - 350N^3 - 300N^2 - 208N - 144, \]  
\[ Q_8(N) = 873N^{14} + 8298N^{13} + 29743N^{12} + 38892N^{11} - 42545N^{10} - 211766N^9 - 227439N^8 + 95376N^7 + 573704N^6 + 942576N^5 + 995168N^4 + 776576N^3 + 527232N^2 + 232704N + 48384, \]  
\[ Q_9(N) = 32N^9 - 936N^8 + 6448N^7 + 55208N^6 + 126160N^5 + 61760N^4 - 53152N^3 - 25024N^2 - 32256N - 13824, \]  
\[ Q_{10}(N) = 7856N^{10} + 84672N^9 + 377648N^8 + 985568N^7 + 1395456N^6 + 470688N^5 - 1183712N^4 - 1180224N^3 - 182528N^2 - 42752N + 13824, \]  
\[ Q_{11}(N) = 60N^9 + 360N^8 + 584N^7 - 128N^6 - 204N^5 - 2440N^4 - 976N^3 - 192N^2 + 896N + 384, \]  
\[ Q_{12}(N) = 28776N^{15} + 356112N^{14} + 1896088N^{13} + 5538320N^{12} + 9112264N^{11} + 6793968N^{10} - 3019528N^9 - 11879520N^8 - 11673088N^7 - 6450992N^6 - 3726976N^5 - 2248128N^4 - 183296N^3 + 268032N^2 + 147456N + 27648, \]  
\[ Q_{13}(N) = 464N^8 - 15616N^7 - 38112N^6 + 27776N^5 + 146064N^4 + 119552N^3 + 109312N^2 + 86016N + 6208, \]  
\[ Q_{14}(N) = 456N^{11} + 4376N^{10} + 11328N^9 - 3184N^8 - 54552N^7 - 111720N^6 - 155376N^5 - 251072N^4 - 312192N^3 - 222464N^2 - 135936N - 41472, \]  
\[ Q_{15}(N) = 168N^8 + 672N^7 + 784N^6 - 3192N^5 - 5600N^4 - 7168N^3 - 7188N^2 - 4480N - 2688, \]  
\[ Q_{16}(N) = 90N^{11} + 630N^{10} + 1592N^9 + 1260N^8 - 1934N^7 - 8218N^6 - 15524N^5 - 23944N^4 - 26752N^3 - 18400N^2 - 11328N - 3456, \]  
\[ Q_{17}(N) = 15777N^{17} + 186525N^{16} + 879391N^{15} + 1874085N^{14} + 575913N^{13} - 5568833N^{12} - 10465411N^{11} - 2970289N^{10} + 11884298N^9 + 12640320N^8 - 10343664N^7 - 40750480N^6 - 55711424N^5 - 53947712N^4 - 42534912N^3 - 23256576N^2 - 7865856N - 1244160. \]
We compared \( \alpha^{(3)}_{Qg}(N) \), Eq. (176), to the fixed moments (H.28–H.32) of Ref. [95] and obtained agreement. The anomalous dimension appears in the \( 1/\varepsilon \) term of (174). As all other contributions to this term are known, the anomalous dimension can be obtained by comparing with the \( 1/\varepsilon \) term of the present computation. The following expression for \( \gamma^{(2)}_{qg}(N) \) is obtained:

\[
\gamma^{(2)}_{qg} = \frac{T^2 n_f}{(N+1)(N+2)} \left\{ C_A \left( (N^2 + N + 2) \left( \frac{128}{3N} S_{2,1} + \frac{32}{9N} S_1 + \frac{128}{3N} S_{-3} \right) + \frac{64}{9N} S_3 - \frac{32}{3N} S_2 S_1 \right) - \frac{128(5N^2 + 8N + 10)}{9N} S_{-2} - \frac{64(5N^4 + 26N^3 + 47N^2 + 43N + 20)}{9N(N+1)(N+2)} S_2 - \frac{64(5N^4 + 20N^3 + 41N^2 + 49N + 20)}{9N(N+1)(N+2)} S_1^2 + \frac{64Q_{18}(N)}{27N(N+1)^2(N+2)^2} S_1 + \frac{16Q_{19}(N)}{27(N-1)N^4(N+1)^3(N+2)^3} \right\} + C_F \left\{ \frac{-32(N^2 + N + 2)}{9N} S_1^3 - \frac{320(N^2 + N + 2)}{9N} S_3 - \frac{32(N^2 + N + 2)}{3N} S_1 S_2 + \frac{32(5N^2 + 3N + 2)}{3N^2} S_2 + \frac{32(10N^3 + 13N^2 + 29N + 6)}{9N^2} S_1^2 - \frac{32(47N^4 + 145N^3 + 426N^2 + 412N + 120)}{27N^2(N+1)} S_1 + \frac{4Q_{20}(N)}{27(N-1)N^5(N+1)^4(N+2)^3} \right\} ,
\]

\( Q_{18}(N) = 19N^6 + 124N^5 + 492N^4 + 1153N^3 + 1362N^2 + 712N + 152 \cdot 10^{(15)} \)

\( Q_{19}(N) = 165N^{12} + 1485N^{11} + 5194N^{10} + 8534N^9 + 3557N^8 - 8899N^7 + 10364N^6 + 6800N^5 + 25896N^4 + 30864N^3 + 19904N^2 + 7296N + 1152 \cdot 10^{(16)} \)

\( Q_{20}(N) = 99N^{14} + 990N^{13} + 4925N^{12} + 17916N^{11} + 46649N^{10} + 72446N^9 + 32283N^8 - 95592N^7 - 267524N^6 - 479472N^5 - 586928N^4 - 455168N^3 - 269760N^2 - 122112N - 27648 \cdot 10^{(17)} \)

It agrees with the moments (H.1-H.5), [89,90,92,94,95]. Due to the algebraic compactification we obtain a lower number of harmonic sums \( S_a(N) \) if compared to Ref. [94], and agree with [201].
8.2 The pure-singlet contribution $A_{Qq}^{PS,(3)}$

The general structure of the pure-singlet contribution $A_{Qq}^{PS,(3)}$ is, [95],

$$A_{Qq}^{PS,(3)} = \left( \frac{m^2}{\mu^2} \right)^{3\varepsilon/2} \left[ \frac{\hat{\gamma}_{qq}^{(0)} \hat{\gamma}_{qq}^{(0)}}{6\varepsilon^3} \left( \gamma_{qq}^{(0)} - \gamma_{qq}^{(0)} + 6\beta_0 + 16\beta_{0,0,Q} \right) + \frac{1}{\varepsilon^2} \left( -\frac{4\hat{\gamma}_{qq}^{(1),PS}}{3} \right) \left[ \hat{\beta}_0 + \hat{\beta}_{0,0,Q} \right] 
- \frac{\gamma_{qq}^{(0)} \hat{\gamma}_{qq}^{(1)}}{3} + \frac{\gamma_{qq}^{(0)} \hat{\gamma}_{qq}^{(1)}}{6} \left( 2\hat{\gamma}_{qq}^{(0)} - \hat{\gamma}_{qq}^{(1)} \right) + \delta m_1^{(-1)} \hat{\gamma}_{qq}^{(0)} \hat{\gamma}_{qq}^{(0)} \right] + \frac{1}{\varepsilon} \left( \frac{\hat{\gamma}_{qq}^{(2),PS}}{3} - n_f \hat{\gamma}_{qq}^{(2),PS} \right) 
+ \delta m_1^{(0)} \hat{\gamma}_{qq}^{(0)} \hat{\gamma}_{qq}^{(0)} - \delta m_1^{(-1)} \hat{\gamma}_{qq}^{(1),PS} \right] + a_{Qq}^{PS,(3)} \right] \right). \tag{198}$$

In this process the photon couples to the heavy quark line. Summing the individual results of the different diagrams (D.201–D.206) weighted by their respective multiplicities yields

$$A_{Qq}^{PS,(3)} = \frac{T_F^2 n_f C_F}{N^2(1+N)(2+N)(1+N)^2} \left\{ -\frac{1}{\varepsilon^3} \frac{256}{9} (N^2 + N + 2)^2 
+ \frac{1}{\varepsilon^2} \left[ -\frac{128}{9} (N^2 + N + 2)^2 S_1 + \frac{128}{27} \frac{Q_{21}(N)}{N(1+N)(2+N)} \right] 
+ \frac{1}{\varepsilon} \left[ (N^2 + N + 2)^2 \left( -\frac{416}{9} S_2 - \frac{32}{9} S_1^2 - \frac{32}{3} S_2 \right) + \frac{64}{27} \frac{Q_{21}(N)}{N(1+N)(2+N)} S_1 - \frac{64}{81} \frac{Q_{22}(N)}{N^2(1+N)^2(2+N)^2} \right] \right\} 
+ a_{Qq}^{PS,(3)}. \tag{199}$$

The constant part is given by

$$a_{Qq}^{PS,(3)} = \frac{T_F^2 n_f C_F}{N^2(1+N)(2+N)(N-1)} \left\{ (N^2 + N + 2)^2 \left( -\frac{1760}{27} S_3 
- \frac{208}{9} S_2 S_1 - \frac{16}{27} S_1^3 - \frac{16}{3} S_1 \zeta_2 + \frac{224}{9} \zeta_3 \right) 
+ \frac{208}{27} \frac{Q_{21}(N)}{N(1+N)(2+N)} S_2 + \frac{16}{27} \frac{Q_{21}(N)}{N(1+N)(2+N)} S_1^2 
+ \frac{16}{9} \frac{Q_{21}(N)}{N(1+N)(2+N)} S_2 - \frac{32}{81} \frac{Q_{22}(N)}{N^2(1+N)^2(2+N)^2} S_1 
+ \frac{32}{243} \frac{Q_{23}(N)}{N^3(1+N)^3(2+N)^3} \right\}, \tag{200}$$

with
\[ Q_{21}(N) = 8 N^7 + 37 N^6 + 68 N^5 - 11 N^4 - 86 N^3 - 56 N^2 - 104 N - 48, \quad (201) \]
\[ Q_{22}(N) = +25 N^{10} + 176 N^9 + 417 N^8 + 30 N^7 - 20 N^6 + 1848 N^5 + 2244 N^4 + 1648 N^3 + 3040 N^2 + 2112 N + 576, \quad (202) \]
\[ Q_{23}(N) = 158 N^{13} + 1663 N^{12} + 7714 N^{11} + 23003 N^{10} + 56186 N^9 + 89880 N^8 + 59452 N^7 - 8896 N^6 - 12856 N^5 - 24944 N^4 - 84608 N^3 - 77952 N^2 - 35712 N - 6912, \quad (203) \]

agreeing with the moments (H.33–H.38) from [95].

### 8.3 The pure-singlet contribution $\hat{A}_{qq,Q}^{(3)}$

The analytic structure for this OME, [95], is given by

\[
\hat{A}_{qq,Q}^{(3), PS} = n_f \left( \frac{m^2}{\mu^2} \right)^{3 \varepsilon/2} \left[ \frac{2 \hat{\gamma}_{qq}^{(0)} \hat{\gamma}_{qq}^{(0)} \beta_{0,Q}}{3 \varepsilon^3} + \frac{1}{3 \varepsilon^2} \left( 2 \hat{\gamma}_{qq}^{(1), PS} \beta_{0,Q} + \hat{\gamma}_{qq}^{(0)} \hat{\gamma}_{qq}^{(1)} \right) \right. \\
+ \left. \frac{1}{\varepsilon} \left( \frac{\hat{\gamma}_{qq}^{(2), PS}}{3} + \hat{\gamma}_{qq}^{(0)} a_{qq,Q}^{(2)} - \frac{\hat{\gamma}_{qq}^{(0)} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \zeta_2}{4} \right) + \frac{a_{qq,Q}^{(3), PS}}{n_f} \right]. \quad (204)
\]

For this OME we computed the complete result, since no other color factors than $T_F^2 n_f C_F$ contribute in this case. The matrix element corresponds to the pure-singlet term in which the photon couples to a massless fermion line. One obtains

\[
A_{qq,Q}^{PS,(3)} = \frac{T_F^2 n_f C_F}{N^2(1 + N)^2(2 + N)(N - 1)} \left\{ \frac{-1}{\varepsilon^3} \frac{256}{9} (N^2 + N + 2)^2 \\
+ \frac{1}{\varepsilon^2} \left[ \frac{256}{9} (N^2 + N + 2)^2 S_1 - \frac{128}{27} \frac{Q_{24}(N)}{N(2 + N)(1 + N)} \right] \\
+ \frac{1}{\varepsilon} \left[ (N^2 + N + 2)^2 \left( -\frac{128}{9} S_2 - \frac{128}{9} S_1^2 - \frac{32}{3} \zeta_2 \right) \right. \\
\left. + \frac{128}{27} \frac{Q_{24}(N)}{N(2 + N)(1 + N)} S_1 - \frac{64}{81} \frac{Q_{25}(N)}{N^2(2 + N)^2(1 + N)^2} \right\} \\
+ a_{qq,Q}^{PS,(3)}, \quad (205)
\]
with the constant part

\[
a_{qq,PS}^{(3)} = \frac{T_F^2 n_f C_F}{N^2(-1+N)(2+N)(1+N)^2} \left\{ (N^2 + N + 2)^2 \left( \frac{256}{27} S_3 + \frac{128}{9} S_2 S_1 \right) + \frac{128}{27} S_1^3 + \frac{32}{3} S_1 \zeta_2 + \frac{224}{9} \zeta_3 \right\} - \frac{64}{27} \frac{Q_{24}(N)}{N(2+N)(1+N)} S_2^2
\]

\[
- \frac{64}{27} \frac{Q_{24}(N)}{N(2+N)(1+N)} \zeta_2
\]

\[
+ \frac{64}{81} \frac{Q_{25}(N)}{N^2(2+N)^2(1+N)^2} S_1 - \frac{32}{243} \frac{Q_{26}(N)}{N^3(2+N)^2(1+N)^3}\right\},
\]

(206)

and

\[
Q_{24}(N) = 16 N^7 + 74 N^6 + 181 N^5 + 266 N^4 + 269 N^3 + 230 N^2 + 44 N - 24,
\]

(207)

\[
Q_{25}(N) = 181 N^{10} + 1352 N^9 + 4737 N^8 + 10101 N^7 + 14923 N^6 + 17085 N^5 + 14133 N^4 + 5944 N^3 + 568 N^2 - 48 N + 144,
\]

(208)

\[
Q_{26}(N) = 2074 N^{13} + 21728 N^{12} + 105173 N^{11} + 311482 N^{10} + 636490 N^9 + 966828 N^8 + 1126568 N^7 + 968818 N^6 + 550813 N^5 + 169250 N^4 + 12104 N^3 - 3408 N^2 - 1008 N - 864,
\]

(209)

agreeing with the fixed moments (H.39-H.45) from [95]. From (198, 199, 204, 205) one may extract the anomalous dimension

\[
\hat{\gamma}_{qg}^{(2),PS} = \frac{C_F T_F^2 n_f}{(N - 1) N^2(N + 1)^2(N + 2)} \left\{ 1 - \frac{32}{3} (N^2 + N + 2)^2 (S_1^2 + S_2) + \frac{64}{9} \frac{Q_{27}(N) S_1}{N(1+N)(2+N)} \right\}
\]

\[
- \frac{64}{27} \frac{Q_{28}(N)}{N^2(1+N)^2(2+N)^2}\right\},
\]

(210)

\[
Q_{27}(N) = 68 N^5 + 37 N^6 + 8 N^7 - 11 N^4 - 114 N^3 - 56 N^2 - 104 N - 48,
\]

(211)

\[
Q_{28}(N) = +52 N^{10} + 392 N^9 + 1200 N^8 + 1353 N^7 - 317 N^6 - 1689 N^5 - 2103 N^4 - 2672 N^3 - 1496 N^2 - 48 N + 144.
\]

(212)

Again we obtain agreement with the fixed moments from [95], Eqs. (H.6-H.12).
8.4 The non-singlet contribution $\hat{A}_{qq,Q}^{NS}$

The following structure is known for the NS contribution:

$$\hat{A}_{qq,Q}^{(3),NS} = \left( \frac{m^2}{\mu^2} \right)^{3\varepsilon/2} \left\{ -\frac{4\gamma_{qq}(0)\beta_{0,Q}}{3\varepsilon^3} (\beta_0 + 2\beta_{0,Q}) + \frac{1}{\varepsilon^2} \left( \frac{2\gamma_{qq}(1)_{NS}\beta_{0,Q}}{3} - \frac{4\gamma_{qq}(1)_{NS}}{3} \right) [\beta_0 + \beta_{0,Q}] 
+ \frac{2\beta_{1,Q}\gamma_{qq}(0)}{3} - 2\delta m_1^{(-1)}\beta_{0,Q}\gamma_{qq}(0) \right\} + \frac{1}{\varepsilon} (\hat{\gamma}_{qq}^{(2),NS})_{320} \left[ \beta_0 + \beta_{0,Q} \right] + \beta_{1,Q}\gamma_{qq}(0)$$

$$+ \frac{\gamma_{qq}(0)\beta_0\beta_{0,Q}\zeta_2}{2} - 2\delta m_1^{(0)}\beta_{0,Q}\gamma_{qq}(0) - \delta m_1^{(-1)}\hat{\gamma}_{qq}^{(1),NS} \right\} + a_{qq,Q}^{(3),NS} \right\}$$

(213)

cf. [95]. We obtain the following result:

$$A_{qq,Q}^{NS,(3)} = T_F^2 n_f C_F \left\{ \frac{1}{\varepsilon^3} \left[ \begin{array}{c} -\frac{512}{27} S_1 + \frac{128}{27} 3 N + 3 N^2 + 2 \frac{3}{(1 + N) N} \\ \frac{256}{27} S_2 - \frac{1280}{81} S_1 + \frac{32}{81} 20 N + 47 N^2 + 6 N^3 + 3 N^4 - 12 \frac{1}{(1 + N)^2 N^2} \\ \frac{1}{\varepsilon} \left[ -\frac{128}{27} S_3 - \frac{64}{9} \zeta_2 S_1 + \frac{640}{81} S_2 + \frac{16}{9} 3 N + 3 N^2 + 2 \frac{3}{(1 + N) N} \zeta_2 - \frac{1280}{27} S_1 \\ + \frac{8}{81} Q_{29}(N) \end{array} \right] \right\} + a_{qq,Q}^{NS,(3)} \right\}$$

(214)

with

$$a_{qq,Q}^{NS,(3)} = T_F^2 n_f C_F \left\{ \frac{64}{27} S_4 + \frac{448}{27} \zeta_3 S_1 + \frac{32}{9} \zeta_2 S_2 - \frac{320}{81} S_3 - \frac{160}{27} \zeta_2 S_1 - \frac{112}{27} \frac{3 N + 3 N^2 + 2}{(1 + N) N} \zeta_3 + \frac{640}{27} S_2 + \frac{4}{27} \frac{20 N + 47 N^2 + 6 N^3 + 3 N^4 - 12}{(1 + N)^2 N^2} \zeta_2 - \frac{55552}{729} S_1 + \frac{2}{729} \frac{Q_{30}(N)}{(1 + N)^4 N^4} \right\}$$

(215)

and

$$Q_{29}(N) = 321 N^6 + 963 N^5 + 1307 N^4 + 833 N^3 + 152 N^2 - 16 N + 24 \right\}, \quad (216)$$

$$Q_{30}(N) = +11751 N^8 + 47004 N^7 + 93754 N^6 + 104364 N^5 + 55287 N^4 + 6256 N^3 - 2448 N^2 - 144 N - 432 . \quad (217)$$

Again the anomalous dimension for the non-singlet case is determined by comparing the $1/\varepsilon$ term of our result to the corresponding term of the general structure. We obtain

$$\hat{\gamma}_{qq}^{(2),NS} = C_F T_F^2 n_f \left\{ \frac{128}{9} S_3 - \frac{640}{27} S_2 - \frac{128}{27} S_1 + \frac{8}{27} \frac{Q_{31}(N)}{N^3(1 + N)^3} \right\}$$

(218)
with
\[ Q_{31}(N) = 51N^6 + 153N^5 + 57N^4 + 35N^3 + 96N^2 + 16N - 24. \]
(219)

For fixed moments \( a_{qq,Q}^{(3),\text{NS}} \) agrees with the values in [95], cf. (H.46–H.60) and the anomalous dimension \( \gamma_{qq}^{(3),\text{NS}} \) with (H.13–H.27), [90, 93, 95].

### 8.5 The non-singlet transversity contribution \( \hat{A}_{qq,Q}^{\text{NS,TR}} \)

The non-singlet transversity OME \( A_{qq,Q}^{\text{NS,TR}} \), cf. Ref. [179], obeys the same general structure as the non-singlet OME \( A_{qq,Q}^{\text{NS}} \), (213). One obtains
\[ A_{qq,Q}^{(3),\text{TR}} = T_{F}^{2}n_{f}C_{F}\left\{ \frac{1}{\varepsilon^{3}} \left[ \frac{128}{9} - \frac{512}{27}S_{1} \right] + \frac{1}{\varepsilon^{2}} \left[ \frac{256}{27}S_{2} - \frac{1280}{81}S_{1} + \frac{32}{27} \right] \right. \]
\[ + \frac{1}{\varepsilon} \left[ -\frac{128}{27}S_{3} - \frac{64}{9}\zeta_{2}S_{1} + \frac{640}{81}S_{2} - \frac{1280}{27}S_{1} + \frac{16}{3}\zeta_{2} \right. \]
\[ \left. + \frac{8(107N^2 + 107N + 8)}{27N(N + 1)} \right\} + a_{qq,Q}^{(3),\text{TR}}, \]  
(220)

with
\[ a_{qq,Q}^{(3),\text{TR}} = T_{F}^{2}n_{f}C_{F}\left\{ \frac{64}{27}S_{1} + \frac{448}{27}\zeta_{3}S_{1} + \frac{32}{9}\zeta_{2}S_{2} - \frac{320}{81}S_{3} - \frac{160}{27}\zeta_{2}S_{1} \right. \]
\[ - \frac{112}{9}\zeta_{3} + \frac{640}{27}S_{2} + \frac{4}{9}\zeta_{2} - \frac{55552}{729}S_{1} \]
\[ \left. + \frac{2(3917N^4 + 7834N^3 + 4157N^2 - 48N - 144)}{243N^2(1 + N)^2} \right\}, \]  
(221)

agreeing with the moments (H.74-H.86) for fixed values of \( N \). Extracting the anomalous dimension from the \( 1/\varepsilon \) term of the OME yields
\[ \hat{\gamma}_{qq}^{(2),\text{TR}} = C_{F}T_{F}^{2}n_{f}\left\{ \frac{128}{9}S_{3} - \frac{640}{27}S_{2} - \frac{128}{27}S_{1} + \frac{8}{9}\left( 17N^2 + 17N - 8 \right) \right\}. \]  
(222)

The results for the anomalous dimensions constitute a first independent check of the result obtained in [179, 203]. It is interesting to note that for this color factor the vector- and tensor operators lead to the same structures in the harmonic sums for \( a_{qq,Q}^{(3)} \) and \( \gamma_{qq}^{(3)} \).

### 8.6 Harmonic Sums

The \( T_{F}^{2}n_{f}C_{F,A} \) contributions at \( O(a_{s}^{3}) \) to the massive operator matrix elements contain nested harmonic sums up to weight \( w = 4 \). This also applies to all individual Feynman diagrams, which we calculated in the Feynman–gauge, cf. Appendix D. In intermediary results generalizations of harmonic sums occur, see Section. 8.7. As has been observed in
the computation of various other physical quantities before, such as anomalous dimensions and massless Wilson coefficients to 3-loop order \cite{93,94,109,201}, unpolarized and polarized massive OMEs to 2–loop order \cite{120,121,123,204}, the polarized and unpolarized Drell-Yan and Higgs-boson production cross section \cite{128}, time-like Wilson coefficients \cite{129}, and virtual- and soft corrections to Bhabha-scattering \cite{130}, the classes of contributing harmonic sums are always the same. For main properties of the nested harmonic sums see Appendix F.3. They depend on the loop-order and the topologies of Feynman diagrams involved.

In the present case the following harmonic sums emerge:

\[
S_1, S_2, S_{-2}, S_3, S_{-3}, S_{2,1}, S_{-2,1}, S_4, S_{-4}, S_{3,1}, S_{-3,1}, S_{-2,2}, S_{2,1,1}, S_{-2,1,1}.
\] (223)

Note that this class, as for the other processes mentioned above, does not contain the index \{-1\}. Moreover, we used the algebraic relations between the harmonic sums, cf. \cite{131}. Furthermore, structural relations exist between harmonic sums, cf. \cite{132,133,202}, which reduce the set (223) further. Here the sums

\[
S_{-2,2}, S_{3,1}
\] (224)

are connected by differential relations w.r.t. their argument \(N\) to other sums of (223). This is also the case for all single harmonic sums \(S_{\pm n}, n \in \mathbb{N}, n > 1\), using both the differentiation and argument-duplication relation, cf. \cite{124}. Due to this \(S_1\) represents the class of all single harmonic sums. I.e. only the six basic harmonic sums

\[
S_1, S_{2,1}, S_{-2,1}, S_{-3,1}, S_{2,1,1}, S_{-2,1,1}
\] (225)

are needed to represent the 3-loop results for the \(T_E n_f C_{F,A}\)-contributions to the OMEs calculated in the present paper. In the final representation we refer to the algebraic basis (223) and consider the basis (225) for a later numerical implementation. We sorted the respective expressions keeping a rational function in \(N\) in front of the harmonic sums (223) and \(\zeta\)-values, like \(\zeta_2\) and \(\zeta_3\).

The harmonic sums emerge from the series–expansion of hypergeometric structures like the Euler \(B\)– and \(\Gamma\)–functions and the Pochhammer–symbols in the (generalized) hypergeometric functions \(\, _pF_q(a_i, b_i; 1)\) in the dimensional parameter \(\epsilon\). This leads to single harmonic sums first, which, through summation, turn into (multiple) zeta values \cite{135} and nested harmonic sums \cite{124,125}. The principle steps on the way from single-scale Feynman diagrams to these structures have been described in Ref. \cite{132}.

8.7 Generalized Harmonic Sums

At 3–loop order the expressions for individual Feynman diagrams are rather large. In Section 7.2 we described how the Feynman parameter integrals which emerge in the present calculation are transformed into nested infinite and finite sums. If these sums
could be computed analytically as a whole only nested harmonic sums would occur in the calculation. However, this is not always possible in practice. Usually the expressions obtained are split into different parts and the sums are then computed. In intermediary steps, depending on the summation methods used, more complicated sum–structures emerge. We will not deal with this aspect here, but only refer to typical structures, which occur in the final result separating the expressions to be summed over into tractable terms of an intermediate size.

Here, so-called generalized harmonic sums occur [205, 206]. They obey the following recursive definition [205]:

\[
\tilde{S}_{m_1,...}(x_1,...; N) = \sum_{i_1}^{N} x_1^{i_1} \sum_{i_2=1}^{i_1-1} x_2^{i_2} \tilde{S}_{m_3,...}(x_3,...; i_2) \\
+ \tilde{S}_{m_1+m_2,m_3,...}(x_1 \cdot x_2, x_3, ...; N).
\]

The sums \(\tilde{S}\) may be reduced to nested harmonic sums for \(x_i \in \{ -1, 1 \}\). In the present calculation the values of \(x_i\) extend to \(\{ -1/2, 1/2, -2, 2 \}\). These sums occur in ladder like structures, cf. [109, 180, 195], but may also emerge, if contributions to 3–loop Feynman diagrams containing a 2-point insertion, are separated into various terms. They were even observed in case of massive 2-loop graphs of the type [121] if large expressions are arbitrarily separated, cf. [195]. The weight of these sums can reach \(w = 5\) intermediary, depending on the \(\varepsilon\)–structure of the contribution, although only \(w = 4\) sums will emerge in the final results. Examples for these sums are:

\[
\tilde{S}_1(1/2; N), \quad \tilde{S}_2(-2; N), \quad \tilde{S}_{2,1}(-1, 2; N), \quad \tilde{S}_{3,1}(-2, -1/2; N),
\]

\[
\tilde{S}_{1,1,1,2}(-1, 1/2, 2, -1; N), \quad \tilde{S}_{2,3}(-2, -1/2; N),
\]

\[
\tilde{S}_{2,2,1}(-1, -1/2, 2; N), \quad \text{etc.}
\]

The algebraic and structural relations for these sums are worked out in Ref. [206]. Similar to the case of harmonic sums, corresponding basis representations are obtained. These relations were provided in a code used in the present calculation. They finally lead to the reduction of the results for the individual diagrams to a representation just in terms of nested harmonic sums. In Appendix G one of the typical lengthy nested sums, which also contains the generalized harmonic sums, is shown.
In the present work a first contribution to the computation of the massive Wilson coefficients of the deep–inelastic structure function \( F_2(x,Q^2) \) for unpolarized charged lepton–nucleon scattering at 3–loop order for general values of the Mellin variable \( N \) in the region \( Q^2 \gtrsim 10 \cdot m^2 \) has been made. Since the corresponding massless Wilson coefficients are known, cf. [109], only the massive operator matrix elements remain to be calculated. A series of fixed Mellin moments for all contributing OMEs has been computed before, Refs. [95,179]. Here, we extend this work to general values of \( N \), calculating a very large class of terms for \( A_{Qg}^{(3)}(N) \) and all contributions to \( A_{qg,Q}^{PS,(3)}(N) \), \( A_{NS,(3)}^{PS}(N) \), \( A_{NS,TR}^{(3)}(N) \) for the color factors \( T_{2,F}^{2,C_F} \) and \( T_{2,F}^{2,C_A} \). The complete results on \( A_{Qg}^{(3)}(N) \) were obtained in a larger team and will be given, including \( A_{qg,Q}^{(3)}(N) \), in [180] in detail.

The present calculation is a first step within a larger programme to compute all topologies contributing to the massive OMEs, including those which define heavy–light quark transitions in the variable flavor number scheme. Due to the large heavy flavor contributions of \( O(25–30\%) \) to the nucleon structure functions the experimental precision of the DIS World Data requires these calculations, both to extract the different parton distribution functions and to measure the strong coupling constant \( \alpha_s(M_Z^2) \) at highest possible precision. The knowledge of these quantities is instrumental for precise measurements at the LHC. \( \alpha_s(M_Z^2) \) is furthermore one of the central parameters in physics.

The present calculation built technically on a method to compute the Feynman–integrals, containing one massive line, directly, i.e. avoiding traditional methods, as integration-by-parts and related techniques. Those usually lead to a large proliferation of terms compared to the compact results being finally obtained. Instead we referred to representations in terms of generalized hypergeometric functions. They occur as the analytic result of the Feynman parameter integrals. Due to this the expansion in the dimensional parameter \( \varepsilon \) can be uniquely performed in an elegant way. At the same time, various significant simplifications of intermediary results are possible choosing particularly this representation. In the end, a small number of nested finite and infinite sums over hypergeometric terms equipped with Beta-functions and harmonic sums has to be performed. In the present calculation up to triple sums occurred. The main technical work to be performed consisted in finding these representation by means of computer algebra for the contributing graphs in a partly automated way. Intermediary very large expressions had to be handled and corresponding codes based on the systems FORM and MAPLE had to be designed.

In the present case the final sums, compared to foregoing massless computations of other groups at 3–loops, cf. e.g. [93,94], turn out to be much more involved due to the the increased nesting in the massive case. Moreover, it has been unclear whether the usual nested harmonic sums form a frame to express all the intermediary results. This had to be found out using strict mathematical methods based on the construction of sum– and product fields. The corresponding software Sigma [142,143] could be used for this purpose. Indeed, it turned out that in the intermediary results the algebra of harmonic sums is to small to describe the corresponding terms and generalized harmonic sums had to be invoked. The methods used would have been pointing to other more general structures also, if contributing. Thus this method is indispensable in exploring new territories in higher order quantum-field theoretic calculations. The present work triggered mathematical research to find all relations for this new class of functions, cf. [206], which
will help to make the codes being used at present even more efficient.

The major new results of the present work are the constant parts of the unrenormalized massive OMEs at 3–loop order for general values of N, \( a^{(3)}_{ij}(N) \) in \( O(T_F^2 n_f C_F, A) \). Furthermore, the corresponding contributions to the 3-loop anomalous dimensions in the vector– and transversity case are obtained. In this way, a first independent recalculation of these important quantities given in [93, 94, 203] before, was performed using very different methods. Here the anomalous dimensions are computed in the massive case. We compared the present results mutually with all the available fixed Mellin moments in the literature and find agreement. In case of the anomalous dimensions the comparison could be performed for the general expressions. The representation we gave, however, is more compact, since we applied the algebraic relations between harmonic sums.

The final results for the matrix elements \( a^{(3)}_{ij}(N) \) and the 3-loop anomalous dimensions \( \hat{\gamma}^{(2)}_{ij}(N) \) are given in harmonic sums only. All generalized harmonic sums cancel already at the level of the individual diagrams. The complexity of harmonic sums determining the present results is maximally six for the \( a^{(3)}_{ij}(N) \) and two for \( \hat{\gamma}^{(2)}_{ij}(N) \) at \( O(T_F^2 n_f C_F, A) \), using also the structural relations, Ref. [132]. This situation is comparable to the case of all massive OMEs at 2–loop order expanded in the dimensional parameter to \( O(\varepsilon) \), cf. [121]. However, the present calculation, at 3–loop order, has been by far more complex and had to pass much more sophisticated structures intermediary. It is interesting to note that the structure w.r.t. harmonic sums for the vector– and tensor flavor non-singlet operators concerning both the matrix elements \( a^{(3)}_{ij}(N) \) and the contributions to the anomalous dimensions \( \hat{\gamma}^{(2)}_{ij}(N) \) are the same for the terms given by the harmonic sums in case at the present color factors.

The present calculations unraveled the relevance of hypergeometric structures in computing Feynman integrals in general. They are given in the present by the generalized hypergeometric functions emerging. Likewise, the finite and infinite sums had to be performed over hypergeometric summands, equipped with products out of (generalized) harmonic sums.

The present work constitutes a first step to explore the general structure of single scale massive observables in QCD at the 3–loop level, which probably bears a rich host of yet unexplored structures. They form an interesting topic to be studied in the future to understand the final simplicity of seemingly complex problems at the higher loop level in Quantum Field Theories such as Quantum Chromodynamics, and hopefully finally the yet unknown reason for that.
10 Appendix
A Conventions

We use natural units

\[ \hbar = 1, \quad c = 1, \quad \varepsilon_0 = 1, \quad (A.1) \]

where \( \hbar \) denotes Planck’s constant, \( c \) the vacuum speed of light and \( \varepsilon_0 \) the permittivity of vacuum. The electromagnetic fine–structure constant \( \alpha \) is given by

\[ \alpha = \alpha' (\mu^2 = 0) = \frac{e^2}{4\pi\varepsilon_0hc} = \frac{e^2}{4\pi} \approx \frac{1}{137.03599911(46)}. \quad (A.2) \]

In this convention, energies and momenta are given in the same units, electron volt (eV).

The space–time dimension is taken to be \( D = 4 + \varepsilon \) and the metric tensor \( g_{\mu\nu} \) in Minkowski–space is defined as

\[ g_{00} = 1, \quad g_{ii} = -1, i = 1 \ldots D - 1, \quad g_{ij} = 0, i \neq j. \quad (A.3) \]

Einstein’s summation convention is used, i.e.

\[ x^\mu y^\mu := \sum_{\mu=0}^{D-1} x_\mu y_\mu. \quad (A.4) \]

Bold–faced symbols represent \((D - 1)\)–dimensional spatial vectors:

\[ x = (x_0, x). \quad (A.5) \]

If not stated otherwise, Greek indices refer to the \( D \)–component space–time vector and Latin ones to the \( D - 1 \) spatial components only. The dot product of two vectors is defined by

\[ p.q = p_0q_0 - \sum_{i=1}^{D-1} p_iq_i. \quad (A.6) \]

The \( \gamma \)–matrices \( \gamma_\mu \) are taken to be of dimension \( D \) and fulfill the anti–commutation relation

\[ \{ \gamma_\mu, \gamma_\nu \} = 2g_{\mu\nu}. \quad (A.7) \]

It follows that

\[ \gamma_\mu \gamma^\mu = D \quad (A.8) \]

\[ \text{Tr} (\gamma_\mu \gamma_\nu) = 4g_{\mu\nu} \quad (A.9) \]

\[ \text{Tr} (\gamma_\mu \gamma_\nu \gamma_\alpha \gamma_\beta) = 4[g_{\mu\nu}g_{\alpha\beta} + g_{\mu\beta}g_{\nu\alpha} - g_{\mu\alpha}g_{\nu\beta}] \quad (A.10) \]

The slash–symbol for a \( D \)–momentum \( p \) is defined by

\[ p^\mu := \gamma_\mu p^\mu. \quad (A.11) \]
The conjugate of a bi-spinor $u$ of a particle is given by

$$\bar{u} = u^\dagger \gamma_0 ,$$  \hspace{1cm} (A.12)

where $\dagger$ denotes Hermitian and $\ast$ complex conjugation, respectively. The bi-spinors $u$ and $v$ fulfill the free Dirac-equation,

$$\begin{align*}
(p^\mu - m)u(p) &= 0 , \quad \bar{u}(p)(p^\mu - m) = 0 \quad \text{(A.13)} \\
(p^\mu + m)v(p) &= 0 , \quad \bar{v}(p)(p^\mu + m) = 0 \quad \text{(A.14)}
\end{align*}$$

Bi-spinors and polarization vectors are normalized to

$$\sum_{\sigma} u(p, \sigma) \bar{u}(p, \sigma) = p^\mu + m \quad \text{(A.15)}$$

$$\sum_{\sigma} v(p, \sigma) \bar{v}(p, \sigma) = p^\mu - m \quad \text{(A.16)}$$

$$\sum_{\lambda} \epsilon^{\mu}(k, \lambda) \epsilon^{\nu}(k, \lambda) = -g^{\mu\nu} \quad \text{(A.17)}$$

where $\lambda$ and $\sigma$ represent the spin.

The commonly used caret “$\hat{}$” to signify an operator, e.g. $\hat{O}$, is omitted if confusion is not to be expected.

The gauge symmetry group of QCD is the Lie–Group $SU(3)_c$. We consider the general case of $SU(N_c)$. The non–commutative generators are denoted by $t^a$, where $a$ runs from 1 to $N_c^2 - 1$. The generators can be represented by Hermitian, traceless matrices, [158]. The structure constants $f^{abc}$ and $d^{abc}$ of $SU(N_c)$ are defined via the commutation and anti–commutation relations of its generators, [160],

$$[t^a, t^b] = if^{abc}t^c \quad \text{(A.18)}$$

$$\{t^a, t^b\} = d^{abc}t^c + \frac{1}{N_c} \delta_{ab} \quad \text{(A.19)}$$

The indices of the color matrices, in a certain representation, are denoted by $i, j, k, l, ...$

The color invariants most commonly encountered are

$$\begin{align*}
\delta_{ab} C_A &= f^{acd} f^{bcd} \quad \text{(A.20)} \\
\delta_{ij} C_F &= t^a_{ii} t^a_{ij} \quad \text{(A.21)} \\
\delta_{ab} T_F &= t^a_{ik} t^b_{ki} \quad \text{(A.22)}
\end{align*}$$

These constants evaluate to

$$C_A = N_c \ , \ C_F = \frac{N_c^2 - 1}{2N_c} \ , \ T_F = \frac{1}{2} \quad \text{(A.23)}$$

At higher loops, more color–invariants emerge. At 3–loop order, one additionally obtains

$$d^{abc} d_{abc} = (N_c^2 - 1)(N_c^2 - 4)/N_c \quad \text{(A.24)}$$

In case of $SU(3)_c$, $C_A = 3 \ , \ C_F = 4/3 \ , \ d^{abc} d_{abc} = 40/3$ holds.
B Feynman Rules

The Feynman rules can be derived, as in any renormalizable Quantum Field theory, from the path integral representation [207–210]. For the QCD Feynman rules, Figure 14, we follow Ref. [160], cf. also Refs. [211, 212]. $D$–dimensional momenta are denoted by $p_i$ and Lorentz-indices by Greek letters. Color indices are $a, b, ...$ and $i, j$ are indices of the color matrices. Solid directed lines represent fermions, wavy lines gluons and dashed lines ghosts. Arrows denote the direction of the momenta. A factor $(-1)$ has to be included for each closed fermion– or ghost loop.

![Feynman rules of QCD](image)

Figure 14: Feynman rules of QCD.
The Feynman rules for the quarkonic composite operators are given in Figure 15. Up to \( O(g^2) \) they can be found in Ref. [81] and also in [213]. Note that the \( O(g) \) term in the former reference contains a typographical error. In Ref. [95] these rules were checked and agree up to normalization factors, which may be due to different conventions. There also the new rule with three external gluons was given. The terms \( \gamma_\pm \) refer to the unpolarized \((+\) and polarized \((-\) case, respectively. Gluon momenta are taken to be incoming.

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

\[
g^{\mu}_{ji} N \gamma_\pm \sum_{j=0}^{N-2} (\Delta \cdot p_1)^j (\Delta \cdot p_2)^{N-2-j} , \quad N \geq 2
\]

\[
g^{\mu \nu \sigma}_{ji} \sum_{j=0}^{N-3} \sum_{l=j+1}^{N-2} (\Delta p_1)^{j} (\Delta p_2)^{N-l-2} \left[ (t^{ab}c)_{ji}(\Delta p_1 + \Delta p_4)^{l-j-1} + (t^{b\nu a}c)_{ji}(\Delta p_1 + \Delta p_4)^{l-j-1} \right] , \quad N \geq 3
\]

\[
g^{\mu \nu \sigma}_{ji} \sum_{j=0}^{N-4} \sum_{l=j+1}^{N-3} \sum_{m=l+1}^{N-2} (\Delta p_1)^{j} (\Delta p_2)^{N-m-2} \left[ (t^{ab}c)_{ji}(\Delta p_4 + \Delta p_5 + \Delta p_1)^l \right] , \quad N \geq 4
\]

\[
\gamma_+ = 1 , \quad \gamma_- = \gamma_5 . \quad \text{For transversity, one has to replace: } \Delta \gamma_\pm \rightarrow \sigma^{\mu\nu} \Delta_\nu .
\]

Figure 15: Feynman rules for quarkonic composite operators. \( \Delta \) denotes a light-like 4-vector, \( \Delta^2 = 0 \); \( N \) is a suitably large positive integer, Ref. [95]
C  D-dimensional integrals

In the calculation of the $D$-dimensional loop integrals [214–216], $D = 4 + \varepsilon$, we perform first a Wick-rotation to Euclidean momenta

$$\prod_{i=1}^{M} \frac{d^D k_i}{(2\pi)^D} f\left(k_i\right) \prod_{i=1}^{M} \frac{1}{(k_i^2 - m_i^2)^{a_i}} = (-1)^{-\sum_{i=1}^{M} a_i} \prod_{i=1}^{M} \frac{d^D k_i}{(2\pi)^D} f\left(-k_i\right) \times \prod_{i=1}^{M} \frac{1}{(-k_i^2 - m_i^2)^{a_i}},$$

with $\forall a_i \in \mathbb{N}$. One obtains the following Euclidean integrals, where, cf. [160],

$$k_E^2 = k_0^2 + k^2,$$

$$\int \frac{d^D k}{(2\pi)^D} \frac{(k^2)^r}{(k^2 - \varphi)^m} = i(-1)^{(r-m)} \int \frac{d^D k_E}{(2\pi)^D} \frac{(k_E^2)^r}{(k_E^2 + \varphi)^m} = i(-1)^{(r-m)} \frac{\Gamma(r+D/2)}{\Gamma(r+D/2)} \frac{\Gamma(m-r-D/2)}{\Gamma(D/2)} \varphi^{r-m+D/2},$$

$$m, r \in \mathbb{N}$$

(C.1)

$$\int \frac{dDk}{D} k^2 f(k^2) = \frac{g^{\alpha_1 \alpha_2}}{D} \int \frac{dDk}{D} k^2 f(k^2)$$

(C.2)

$$\int \frac{dDk}{D} \frac{k_1^\alpha k_2^\alpha}{D^2 + 2D} f(k^2) = \int \frac{dDk}{D} k^4 f(k^2)$$

(C.3)

$$\int \frac{dDk}{D} \frac{k_1^\alpha k_2^\alpha k_3^\alpha k_4^\alpha k_5^\alpha k_6^\alpha}{D^3 + 6D^2 + 8D} \int \frac{dDk}{D} k^6 f(k^2),$$

(C.4)

with

$$P_6(g^{\alpha_1 \alpha_2}) = g^{\alpha_1 \alpha_2} \left[ g^{\alpha_3 \alpha_4} g^{\alpha_5 \alpha_6} + g^{\alpha_3 \alpha_5} g^{\alpha_4 \alpha_6} + g^{\alpha_3 \alpha_6} g^{\alpha_4 \alpha_5} \right]$$

$$+ g^{\alpha_1 \alpha_3} \left[ g^{\alpha_2 \alpha_4} g^{\alpha_5 \alpha_6} + g^{\alpha_2 \alpha_5} g^{\alpha_4 \alpha_6} + g^{\alpha_2 \alpha_6} g^{\alpha_4 \alpha_5} \right]$$

$$+ g^{\alpha_1 \alpha_4} \left[ g^{\alpha_2 \alpha_3} g^{\alpha_5 \alpha_6} + g^{\alpha_2 \alpha_5} g^{\alpha_3 \alpha_6} + g^{\alpha_2 \alpha_6} g^{\alpha_3 \alpha_5} \right]$$

$$+ g^{\alpha_1 \alpha_5} \left[ g^{\alpha_2 \alpha_4} g^{\alpha_5 \alpha_6} + g^{\alpha_2 \alpha_6} g^{\alpha_4 \alpha_5} \right] + g^{\alpha_1 \alpha_6} \left[ g^{\alpha_3 \alpha_4} g^{\alpha_5 \alpha_6} + g^{\alpha_3 \alpha_5} g^{\alpha_4 \alpha_6} + g^{\alpha_3 \alpha_6} g^{\alpha_4 \alpha_5} \right]$$

(C.5)

and

$$\int \frac{dDk}{D} \prod_{i=1}^{2M+1} k_i^\alpha f(k^2) = 0.$$  

(C.6)

For each loop integral a universal factor

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

(C.7)
emerges, where \( \gamma_E \) denotes the Euler–Mascheroni constant

\[
\gamma_E = \lim_{k \to \infty} \left[ \sum_{l=1}^{k} \frac{1}{l} - \ln(k) \right].
\] (C.8)

The factors \( S_\varepsilon \) are kept separately and are not expanded in \( \varepsilon \). In the \( \overline{\text{MS}} \)-scheme \([97]\) they are set to \( S_\varepsilon = 1 \) at the end of the calculation.

The \( \Gamma \)-function obeys the relation

\[
\Gamma(1 + \varepsilon) = \exp \left[ -\gamma_E \varepsilon + \sum_{n=2}^{\infty} \frac{(-\varepsilon)^n}{n} \zeta_n \right],
\] (C.9)

with

\[
\zeta_n = \sum_{k=1}^{\infty} \frac{1}{k^n}, \quad n \in \mathbb{N}, \quad n \geq 2,
\] (C.10)

the Riemann \( \zeta \)-function at integer arguments.

We apply the following Feynman parametrization to combine denominators

\[
\frac{1}{A_1 \ldots A_n} = \Gamma(n) \int_0^1 dx_1 \ldots \int_0^1 dx_n \delta \left( \sum_{k=1}^{n} x_k - 1 \right) \frac{1}{(x_1 A_1 + \ldots + x_n A_n)^n},
\] (C.11)

resp.

\[
\frac{1}{A_1^{a_1} \ldots A_n^{a_n}} = \frac{\Gamma \left( \sum_{k=1}^{n} a_k \right)}{\prod_{k=1}^{n} \Gamma(a_k)} \int_0^1 dx_1 \ldots \int_0^1 dx_n \delta \left( \sum_{k=1}^{n} x_k - 1 \right)
\]
\[
\times \frac{\prod_{k=1}^{n} x_k^{a_k-1}}{(x_1 A_1 + \ldots + x_n A_n)^{\left( \sum_{k=1}^{n} a_k \right)}},
\] (C.12)

with \( \forall a_i \in \mathbb{N} \).

The integral over the \( \delta \)-distribution yields

\[
\int_0^1 dx_1 \delta \left( \sum_{k=1}^{n} x_k - 1 \right) = \int_{-\infty}^{+\infty} dx_1 \delta \left( \sum_{k=1}^{n} x_k - 1 \right) \theta \left( 1 - \sum_{k=1}^{n} x_k \right) \prod_{m=1}^{n} \theta(x_m)
\]
\[
= \theta \left( 1 - \sum_{k=1,k \neq l}^{n} x_k \right) \prod_{m=1,m \neq l}^{n} \theta(x_m),
\] (C.13)

where \( \theta(z) \) denotes the Heaviside function

\[
\theta(z) = \begin{cases} 
1, & z \geq 0 \\
0, & z < 0
\end{cases}
\] (C.14)
D Results for the Individual Diagrams

In this appendix we list the results for the individual diagrams contributing to the $O\left(\frac{T^2 N_f C_F}{N^2(N+1)}\right)$ terms in the massive operator matrix elements $A_{Qg}^{(3)}, A_{Qg}^{(3),PS}, A_{qq,Q}^{(3),PS}, A_{qq,Q}^{(3),NS}$ and $A_{qq,Q}^{(3),TR}$. They are all represented in terms of harmonic sums, despite the fact that in intermediate results also generalized harmonic sums occur. No sums beyond $w=4$ contribute. Furthermore, the individual diagrams do not contain sums, which fully cancel in the final result, similar to [120,121]. The individual contributions were compared to the corresponding moments in the calculation Ref. [95, 179]. The common prefactor

$$\hat{a}_s^3 S_3^3 \left(\frac{m^2}{\mu^2}\right)^{3/2} \frac{1 + (-1)^N}{2}$$

has been taken out.

D.1 $\hat{A}_{Qg}$

The results for the individual diagrams contributing to $\hat{A}_{Qg}$ are:

$$\hat{A}_{Qg}^{(3),A_1} = \frac{T^2 N_f C_F}{N^2(N+1)} \left\{ -\frac{1}{\varepsilon^3} \left[ \frac{64(N-1)(N+2)}{9} \right] - \frac{1}{\varepsilon^2} \left[ \frac{64(2N^4 - 5N^3 + 7N^2 + 2N + 3)}{27N(N+1)} \right] + \frac{1}{\varepsilon} \left[ -\frac{32}{3}(N-1)(N+2)S_2 - \frac{8}{3}(N-1)(N+2)\zeta_2 - \frac{32P_1(N)}{81N^2(N+1)^2(N+2)^2} \right] - 16(N-1)(N+2)S_3 + \frac{56}{9}(N-1)(N+2)\zeta_3 - \frac{32(2N^4 - 5N^3 + 7N^2 + 2N + 3)}{9N(N+1)} \right\} \right. \left(\frac{1}{27(N+1)(N+2)} \right)^2 \right\},$$

with

$$P_1(N) = 5N^8 + 26N^7 - 203N^6 - 721N^5 - 1079N^4 - 460N^3 + 269N^2 + 444N + 180,$$

$$P_2(N) = 17N^{11} + 107N^{10} + 824N^9 - 927N^8 - 8904N^7 - 17883N^6 - 19301N^5 - 10193N^4 + 3973N^3 + 15342N^2 + 11052N + 2808.$$

$$\hat{A}_{Qg}^{(3),B_1} = \frac{T^2 N_f C_F}{N} \left\{ \frac{1}{\varepsilon^3} \left[ -\frac{128}{9} S_1 + \frac{128}{9} \right] + \frac{1}{\varepsilon^2} \left[ -\frac{64}{9} S_1^2 + \frac{128}{9} S_2 \right] + \frac{128(4N^2 + 21N + 8)}{27(N+1)(N+2)} S_1 - \frac{64(11N^2 + 51N + 22)}{27(N+1)(N+2)} \right\}.$$
+ \frac{1}{\varepsilon} \left\{ \begin{array}{l} \frac{64}{3} S_{2,1} - \frac{64}{27} S_1^3 + \frac{736}{27} S_3 - \frac{64}{9} S_2 S_1 - \frac{16}{3} \zeta_2 S_1 \\ \frac{64(4N^2 + 21N + 8)}{27(N + 1)(N + 2)} S_2^2 + \frac{64(N^2 - 15N + 2)}{27(N + 1)(N + 2)} S_2 + \frac{16}{3} \zeta_2 \\ - \frac{32P_3(N)}{81N(N + 1)^2(N + 2)^2} S_1 + \frac{32P_4(N)}{81(N + 1)^3(N + 2)^2} \\ - \frac{16}{27} S_4^2 + \frac{32}{9} S_2^2 + \frac{352}{9} S_4 - \frac{128}{27} S_3 S_1 + \frac{112}{9} \zeta_3 S_1 - \frac{64}{3} S_{3,1} + \frac{32}{3} S_{2,1,1} \\ - \frac{32}{9} S_2 S_1^2 - \frac{8}{3} \zeta_2 S_1 + \frac{16}{3} \zeta_2 S_1 - \frac{64}{3} S_{2,1} S_1 + \frac{64(4N^2 + 21N + 8)}{9(N + 1)(N + 2)} S_{2,1} \\ + \frac{64(4N^2 + 21N + 8)}{27(N + 1)(N + 2)} S_2 S_1 + \frac{16(4N^2 + 21N + 8)}{9(N + 1)(N + 2)} \zeta_2 S_1 \\ + \frac{64(4N^2 + 21N + 8)}{81(N + 1)(N + 2)} S_3 - \frac{32(11N^2 + 240N + 22)}{81(N + 1)(N + 2)} S_3 \\ - \frac{112}{9} \zeta_3 - \frac{8(11N^2 + 51N + 22)}{9(N + 1)(N + 2)} \zeta_2 - \frac{8P_5(N)}{81(N + 1)^2(N + 2)^2} S_1^2 \\ - \frac{8P_6(N)}{16P_7(N)} \zeta_2 - \frac{243N(N + 1)^3(N + 2)^3}{16P_7(N)} S_2 + \frac{243N(N + 1)^3(N + 2)^3}{16P_7(N)} S_2 \\ - \frac{16P_8(N)}{243(N + 1)^4(N + 2)^3} \right\} ,
\tag{D.5}
\end{array} \right.

\text{with}

\begin{align*}
P_3(N) & = 88N^5 + 780N^4 + 1873N^3 + 1938N^2 + 892N + 216 , \\
P_4(N) & = 121N^5 + 1126N^4 + 3280N^3 + 3907N^2 + 1792N + 484 , \\
P_5(N) & = 176N^5 + 1614N^4 + 4097N^3 + 4686N^2 + 2324N + 648 , \\
P_6(N) & = 44N^5 + 282N^4 + 2057N^3 + 3966N^2 + 1796N + 648 , \\
P_7(N) & = 824N^7 + 10350N^6 + 46281N^5 + 104256N^4 + 124746N^3 + 77364N^2 + 24952N + 4752 , \\
P_8(N) & = 1187N^7 + 15182N^6 + 70743N^5 + 161517N^4 + 197367N^3 + 137022N^2 + 56836N + 9496 . 
\end{align*}

\begin{align*}
\zeta^{(3),C_1}_{Q_9} = T_F^2 n_f C_F \frac{1}{N} \left\{ \begin{array}{l} \varepsilon^2 \left[ \frac{16(13N^2 + 65N + 6)}{3(N + 2)(N + 3)} \right] \\ + \frac{1}{\varepsilon} \left[ 64S_2 - \frac{4P_9(N)}{3N(N + 1)^2(N + 2)^2(N + 3)} \right] \\ + \frac{96S_3}{(N + 2)(N + 3)} \zeta_2 - \frac{8(13N^3 + 86N^2 + 191N + 102)}{(N + 1)(N + 2)(N + 3)} S_2 \\ + \frac{P_{10}(N)}{3N^2(N + 1)^3(N + 2)^3(N + 3)} \right\} ,
\end{array} \right.
\tag{D.12}
\end{align*}
with

\[
P_9(N) = 91N^6 + 855N^5 + 2481N^4 + 3037N^3 + 1436N^2 - 28N - 48 , \quad (D.13)
\]

\[
P_{10}(N) = 569N^9 + 7152N^8 + 33604N^7 + 79234N^6 + 99271N^5 + 61206N^4
+ 13356N^3 + 584N^2 + 800N + 384 . \quad (D.14)
\]

\[
\hat{A}_{Qg}^{(3),D_1} = \frac{T_F^2 n_f C_F}{N(N + 2)(N + 3)} \left\{ \frac{1}{\varepsilon^2} \left[ \frac{16(N^2 + 5N + 42)}{3} \right] + \frac{1}{\varepsilon} \left[ \frac{16(N + 3)(N^4 + 4N^3 + 41N^2 + 32N + 12)}{3N(N + 1)^2} S_1 - \frac{4P_{11}(N)}{3(N + 1)^3(N + 2)} \right] + 2(N^2 + 5N + 42)\zeta_2 + \frac{8P_{12}(N)}{3N(N + 1)^2} S_1 + \frac{8P_{12}(N)}{3N(N + 1)^2} S_2 - \frac{4P_{13}(N)}{3N(N + 1)^3(N + 2)} S_1 + \frac{P_{14}(N)}{3(N + 1)^4(N + 2)^2} \right\} , \quad (D.15)
\]

with

\[
P_{11}(N) = 7N^6 + 70N^5 + 748N^4 + 2770N^3 + 3961N^2 + 2320N + 588 , \quad (D.16)
\]

\[
P_{12}(N) = N^5 + 7N^4 + 53N^3 + 188N^2 + 141N + 54 , \quad (D.17)
\]

\[
P_{13}(N) = 7N^7 + 70N^6 + 730N^5 + 3340N^4 + 6127N^3 + 5074N^2 + 2340N
+ 504 , \quad (D.18)
\]

\[
P_{14}(N) = 53N^8 + 665N^7 + 7044N^6 + 36078N^5 + 90789N^4 + 122301N^3
+ 93322N^2 + 40780N + 7752 . \quad (D.19)
\]

\[
\hat{A}_{Qg}^{(3),E_1} = T_F^2 n_f \left( C_F - \frac{C_A}{2} \right) \frac{1}{N(N + 1)} \left\{ \frac{1}{\varepsilon^3} \left[ \frac{64(N - 1)}{9(N + 1)} \right] + \frac{1}{\varepsilon^2} \left[ -\frac{32}{9} (4N + 5) S_1 + \frac{16(N - 1)(15N^3 + 47N^2 + 44N + 18)}{27N(N + 1)^2} \right] + \frac{1}{\varepsilon} \left[ -\frac{8(8N^3 + 29N^2 + 41N - 66)}{9(N + 2)(N + 3)} S_1^2 + \frac{8(N - 1)}{3(N + 1)} \zeta_2 \right] - \frac{8(32N^4 + 157N^3 + 310N^2 + 71N - 66)}{9(N + 1)(N + 2)(N + 3)} S_2
+ \frac{8P_{15}(N)}{27N(N + 1)(N + 2)(N + 3)} S_1 - \frac{4P_{16}(N)}{81N^2(N + 1)^3(N + 2)^2(N + 3)} \right\} - \frac{4(16N^3 + 37N^2 + 25N - 258)}{27(N + 2)(N + 3)} S_1^3 - \frac{4}{3} (4N + 5) \zeta_2 S_1 \]

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\[ A_{Qg}^{(3,F_1)} = \frac{1}{T^2 n_f} \left( C_F - \frac{C_A}{2} \right) \left( \frac{1}{(N+1)(N+2)} \right) \left( \frac{1}{\varepsilon^3} \right) \left[ \frac{-512}{9} + \frac{512}{9} S_1 \right] + \frac{1}{\varepsilon^2} \left[ \frac{64}{9} \frac{S_2}{N^2} - \frac{64(4N^2 + 9N + 8)}{9N} S_2 + \frac{128(3N^3 - N^2 + 30N + 12)}{27N^2} S_1 \right. \\
- \left. \frac{128(3N^3 + 2N^2 + 17N + 6)}{27N(N + 1)} \right] + \frac{1}{\varepsilon} \left[ \frac{32}{27} S_1^2 + \frac{64(3N^3 + 20N^2 + 3N + 12)}{27N^2} S_1^2 - \frac{64P_{21}(N)}{81N^2(N + 1)(N + 2)} S_1 \right. \\
+ \frac{64}{3} \zeta_2 S_1 - \frac{32}{9} S_2 S_1 + \frac{64P_{22}(N)}{81N(N + 1)^2(N + 2)} - \frac{64\zeta_2}{3} S_1 \\
+ \frac{64(4N^3 + 87N^2 - 85N - 24)}{27N^2} S_2 - \frac{256(3N^2 + 10N + 6)}{27N} S_3 \\
+ \frac{128(N + 1)(N + 2)}{3N} S_{2,1} \right] - \frac{20}{27} S_1^4 + \frac{8}{3} \zeta_2 S_1^2 - \frac{40}{9} S_2 S_1^2 - \frac{448}{9} \zeta_3 S_1 \right], \quad (D.20) \]
\[
-\frac{160}{27} S_3 S_1 + \frac{64}{3} S_{2,1} S_1 - \frac{4(48 N^2 + 101 N + 96)}{9 N} S_2^2 - \frac{8(4 N^2 + 9 N + 8)}{3 N} \zeta_2 S_2
+ \frac{64}{3} S_{3,1} + \frac{64(3 N^2 + 7 N + 6)}{3 N} S_{2,1,1} - \frac{8(56 N^2 + 169 N + 112)}{9 N} S_4
+ \frac{32(6 N^3 + 61 N^2 - 21 N + 24)}{81 N^2} S_1 + \frac{16(3 N^3 - N^2 + 30 N + 12)}{9 N^2} \zeta_2 S_1
+ \frac{32(6 N^3 + 61 N^2 - 21 N + 24)}{27 N^2} S_2 S_1 - \frac{128(N^3 + 9 N^2 - 10 N - 6)}{9 N^2} S_{2,1}
+ \frac{448}{9} \zeta_3 - \frac{32(9 N^3 - 623 N^2 + 894 N + 276)}{81 N^2} S_3 - \frac{16 P_{23}(N)}{81 N^2 (N + 1)(N + 2)} S_1^2
- \frac{16(3 N^3 + 2 N^2 + 17 N + 6)}{9 N(N + 1)} \zeta_2 - \frac{16 P_{24}(N)}{81 N^2 (N + 1)(N + 2)} S_2
+ \frac{32 P_{25}(N)}{243 N^2 (N + 1)^2(N + 2)^2} S_1 - \frac{32 P_{26}(N)}{243 N(N + 1)^3(N + 2)} \right),
\]

with

\[
P_{21}(N) = 24 N^5 + 196 N^4 + 1047 N^3 + 1748 N^2 + 984 N + 120 ,
\]
\[
P_{22}(N) = 33 N^5 + 364 N^4 + 1462 N^3 + 2543 N^2 + 1904 N + 132 ,
\]
\[
P_{23}(N) = 48 N^5 + 746 N^4 + 2697 N^3 + 2746 N^2 + 1104 N + 240 ,
\]
\[
P_{24}(N) = 124 N^5 + 198 N^4 - 2387 N^3 - 6162 N^2 - 3632 N - 480 ,
\]
\[
P_{25}(N) = 264 N^7 + 4046 N^6 + 21591 N^5 + 52844 N^4 + 74856 N^3 + 66812 N^2 + 30576 N + 264 ,
\]
\[
P_{26}(N) = 363 N^7 + 6758 N^6 + 41285 N^5 + 121235 N^4 + 190235 N^3 + 150758 N^2 + 46964 N + 2904 .
\]

\[
z_{G_1}^{(3),Qg} = \frac{T^2 T_f C_F}{(N + 1)(N + 2)} \left\{ -1 - \frac{1224}{3 \varepsilon^2} + \frac{1}{\varepsilon} \left[ -64 S_2
- \frac{16 (N^2 + 27 N + 38)}{3(N + 1)(N + 2)} S_1 + \frac{8 (65 N^4 + 430 N^3 + 881 N^2 + 608 N + 44)}{3(N + 1)^2(N + 2)^2} \right]
- 96 S_3 - \frac{8 (N^3 + 30 N^2 + 137 N + 144)}{3(N + 1)(N + 2)(N + 3)} S_1^2 - 28 \zeta_2
+ \frac{16(25 N^3 + 150 N^2 + 248 N + 105)}{3(N + 1)(N + 2)(N + 3)} S_2 + \frac{4 P_{27}(N)}{3(N + 1)^2(N + 2)^2(N + 3)} S_1
- \frac{2 P_{28}(N)}{3(N + 1)^3(N + 2)^3(N + 3)} \right\},
\]

with

\[
P_{27}(N) = 13 N^6 + 373 N^5 + 2197 N^4 + 4907 N^3 + 4534 N^2 + 1464 N + 144 ,
\]
\[
P_{28}(N) = 455 N^7 + 5828 N^6 + 29700 N^5 + 77486 N^4 + 111073 N^3 + 87014 N^2 + 35364 N + 6840 .
\]
\[
\begin{align*}
\zeta^{(3), H_1}_{Qg} &= T_{\bar{F}n_f}^2 \left( C_F - \frac{C_A}{2} \right) \frac{1}{N+1} \left\{ \frac{1}{\varepsilon^2} \left[ \frac{320}{9N} S_1 - \frac{128}{3(N+2)} \right] \right. \\
&\quad + \frac{1}{\varepsilon} \left[ \frac{16}{9N(N+2)(N+3)} S_1^2 \right. \\
&\quad - \frac{16}{27N(N+1)(N+2)^2(N+3)} S_1 \\
&\quad - \left. \frac{16P_{29}(N)}{3(N+1)^2(N+2)^3(N+3)} + \frac{16}{9N(N+2)(N+3)} S_2 \right] \\
&\quad - \frac{8(7N^2 - 73N + 150)}{27N(N+2)(N+3)} S_1^3 + \frac{40}{3N} \zeta_{S_2} S_1 \\
&\quad - \frac{8(7N^2 - 73N + 150)}{9N(N+2)(N+3)} S_2 S_1 + \frac{16}{27N(N+2)(N+3)} S_3 + \frac{160}{3N} S_{2,1} \\
&\quad + \frac{4(119N^4 - 962N^3 - 3137N^2 + 3784N + 332)}{27N(N+1)(N+2)^2(N+3)} S_1^2 - \frac{16}{(N+2)} \zeta_2 \\
&\quad - \frac{4P_{30}(N)}{81N(N+1)^2(N+2)^3(N+3)} S_1 \\
&\quad + \frac{8P_{31}(N)}{9(N+1)^3(N+2)^4(N+3)} \\
&\left. \right\}, \quad \text{(D.37)}
\end{align*}
\]

with

\[
\begin{align*}
P_{29}(N) &= 7N^5 + 7N^4 - 203N^3 - 955N^2 + 1604N - 948, \quad \text{(D.38)} \\
P_{30}(N) &= 427N^6 - 10201N^5 - 91517N^4 - 319471N^3 - 556466N^2 \\
&\quad - 463084N - 137784, \quad \text{(D.39)} \\
P_{31}(N) &= 253N^7 + 1884N^6 + 3444N^5 - 9582N^4 - 50265N^3 - 82446N^2 \\
&\quad - 58120N - 13680. \quad \text{(D.40)}
\end{align*}
\]

\[
\begin{align*}
\zeta^{(3), I_1}_{Qg} &= \frac{T_{\bar{F}n_f}^2}{(N+1)(N+2)} \left\{ \\
&\left. \begin{array}{l}
C_F \left\{ \frac{1}{\varepsilon^2} \left[ \frac{32}{3} S_1^2 - \frac{32}{3} S_2 - \frac{128(N+1)}{3N} S_1 + \frac{256}{3} \right] \\
+ \frac{1}{\varepsilon} \left[ \frac{16}{3} S_1^3 + 16S_1S_2 - \frac{64}{3} S_3 + \frac{32(7N+3)}{9N} S_2 - \frac{32(13N-3)}{9N} S_1^2 \\
+ \frac{64}{9N(N+1)} \frac{20N^2 + 37N + 23}{S_1} - \frac{2560}{9} \right] \\
+ \frac{14}{9} S_1^4 + \frac{28}{3} S_2 S_1 + \frac{14}{3} S_2^2 - 64S_{2,1}S_1 - 4\zeta_2 S_2 + 4\zeta_2 S_1^2 + 32S_{3,1}
\end{array} \right. \right\}
\end{align*}
\]
\[
\begin{align*}
&+ \frac{112}{9} S_3 S_1 - 28 S_4 - \frac{16(11N - 5)}{9N} S_1^3 - \frac{16(N + 1)}{N} \zeta_2 S_1 - \frac{16(11N - 5)}{3N} S_2 S_1 \\
&+ \frac{32(19N + 5)}{9N} S_3 - \frac{64(N + 1)}{N} S_{2,1} + \frac{16(179N^2 + 200N + 75)}{27N(N + 1)} S_1^2 + 32 \zeta_2 \\
&- \frac{16(23N^2 + 2N - 75)}{27N(N + 1)} S_2 - \frac{32(274N^3 + 816N^2 + 921N + 325)}{27N(N + 1)^2} S_1 + \frac{16(6N + 5)}{9} S_2 \\
&+ C_A \left\{ \frac{1}{\varepsilon^3} \left[ 1 + \frac{64(N + 4)}{9(N + 2)} S_1 - 16(18N + 13) S_2 S_1 + \frac{80(N + 1)}{3} S_{-2} + \frac{16(54N + 49)}{27} S_3 \right] \\
&+ \frac{1}{\varepsilon^2} \left[ \frac{8(18N + 13)}{9} S_2 S_1 + \frac{80(N + 1)}{3} S_{-2} + \frac{16(54N + 49)}{27} S_3 \right] \\
&- \frac{32(N + 1)}{S_{-2,1}} - \frac{16(3N + 1)}{3} S_{-2,1} - \frac{32(8N^2 + 3N - 14)}{9(N + 2)} S_{-2} \\
&- \frac{16}{27N(N + 1)(N + 2)} S_2 + \frac{16(22N^3 + 69N^2 + 35N - 18)}{27N(N + 1)(N + 2)^2} S_1^2 \\
&- \frac{8(N + 4)}{3(N + 2)} \zeta_2 - \frac{16P_{32}(N)}{81N(N + 1)(N + 2)^2} S_1 + \frac{16P_{33}(N)}{81N(N + 1)^2(N + 2)^3} S_3 \\
&- \frac{13}{27} S_1^4 - \frac{8(9N + 11)}{3} S_{2,1} S_1 - 48(N + 1) S_{-2,1} S_1 + \frac{8(162N + 149)}{27} S_3 S_1 \\
&+ \frac{40(N + 1)}{3} S_{-2} S_1 - \frac{56}{9} \zeta_3 S_1 - \frac{(36N + 73)}{9} S_2^2 + 8(N + 1) \zeta_2 S_{-2} \\
&+ \frac{2(6N + 5)}{3} \zeta_2 S_2 + 8(N + 1) S_{-2} S_2 + 24(N + 1) S_{-2} S_1^2 - \frac{16(9N + 10)}{3} S_{3,1} \\
&+ \frac{48(N + 1)}{3} S_{-2,1,1} + \frac{8(9N + 19)}{3} S_{2,1,1} + \frac{2(228N + 203)}{9} S_4 - 40(N + 1) S_{-3,1} \\
&+ \frac{32(N + 1)}{S_{-2,2}} + \frac{8(65N^3 + 174N^2 + 31N - 90)}{81N(N + 1)(N + 2)} S_1^3 \\
&- \frac{8(72N^4 + 34N^3 - 273N^2 - 157N + 90)}{27N(N + 1)(N + 2)} S_2 S_1 + \frac{4(N^3 + 33N^2 + 74N + 36)}{9N(N + 1)(N + 2)} \zeta_2 S_1 \\
&- \frac{16}{3(N + 2)} S_{-2} S_1 - \frac{8(N + 1)}{3} S_{-4} - \frac{40(8N^2 + 3N - 14)}{9(N + 2)} S_{-3} \\
&+ \frac{56(N + 4)}{9(N + 2)} \zeta_3 + \frac{2(54N + 41)}{9} S_2 S_1^2 - \frac{8(432N^4 + 707N^3 + 111N^2 + 154N + 180)}{81N(N + 1)(N + 2)} S_3 \\
&- \frac{2}{3} \zeta_2 S_1^2 + \frac{16}{3(N + 2)} S_{-2,1} + \frac{8(24N^4 + 35N^3 + 33N^2 + 106N + 72)}{9N(N + 1)(N + 2)} S_{2,1} \\
&- \frac{4P_{34}(N)}{81N(N + 1)^2(N + 2)^2} S_1^2 - \frac{4(7N^3 + 25N^2 + 80N + 80)}{9(N + 1)(N + 2)^2} \zeta_2
\end{align*}
\]
\[\begin{align*}
&+ \frac{64 (13N^4 + 36N^3 + 73N^2 + 153N + 130)}{27(N + 1)(N + 2)^2} S_{-2} + \frac{4P_35(N)}{81N(N + 1)^2(N + 2)^2} S_2 \\
&+ \frac{8P_36(N)}{243N(N + 1)^3(N + 2)^3} S_1 - \frac{8P_37(N)}{243(N + 1)^3(N + 2)^4} \right) \right)
\end{align*}\]
with

\[\begin{align*}
P_{32}(N) &= 173N^5 + 1494N^4 + 4706N^3 + 7191N^2 + 5588N + 1872, \\
P_{33}(N) &= 320N^5 + 2720N^4 + 9797N^3 + 17507N^2 + 15272N + 5216, \\
P_{34}(N) &= 700N^5 + 4572N^4 + 10909N^3 + 12447N^2 + 7624N + 2448, \\
P_{35}(N) &= 312N^6 + 962N^5 + 456N^4 - 2947N^3 - 7203N^2 - 6880N \\
&\quad - 2448, \\
P_{36}(N) &= 3019N^7 + 33159N^6 + 152637N^5 + 388497N^4 + 593193N^3 \\
&\quad + 540399N^2 + 267080N + 52848, \\
P_{37}(N) &= 5041N^7 + 58633N^6 + 293478N^5 + 808539N^4 + 1321572N^3 \\
&\quad + 1281873N^2 + 683576N + 154784.
\end{align*}\]

\[\begin{align*}
\zeta^{(3)}_{\lambda, \mu} \bar{A}_{Qg} &= \frac{T_f^2 m_f C_A}{N^2(N + 1)^2} \left\{ \frac{1}{\varepsilon^3} \left[ \frac{32(N - 3)(2N^2 + N - 4)}{9} \right] \\
&\quad - \frac{16P_{38}(N)}{27(N - 1)N(N + 1)(N + 2)} \\
&\quad + \frac{16}{3} (N - 3)(2N^2 + N - 4)S_2 + \frac{4}{3} (N - 3)(2N^2 + N - 4)\zeta_2 \\
&\quad + \frac{8P_{39}(N)}{81(N - 1)^2N^2(N + 1)^2(N + 2)^2} + 8(N - 3)(2N^2 + N - 4)S_3 \\
&\quad - \frac{2}{9} (N - 3)(2N^2 + N - 4)\zeta_3 - \frac{8P_{38}(N)}{9(N - 1)N(N + 1)(N + 2)} S_2 \\
&\quad - \frac{2P_{38}(N)}{9(N - 1)N(N + 1)(N + 2)} \zeta_2 \\
&\quad - \frac{4P_{40}(N)}{243(N - 1)^3N^3(N + 1)^3(N + 2)^3} \right\},
\end{align*}\]
with

\[\begin{align*}
P_{38}(N) &= 16N^7 - 17N^6 - 209N^5 + 142N^4 - 65N^3 - 629N^2 + 186N \\
&\quad + 216, \\
P_{39}(N) &= 68N^{11} + 75N^{10} - 1715N^9 - 2112N^8 - 3360N^7 + 24N^6 \\
&\quad + 2454N^5 + 11469N^4 - 24037N^3 - 6432N^2 + 4932N + 3024, \\
P_{40}(N) &= 460N^{15} + 1799N^{14} - 11123N^{13} - 40963N^{12} - 38795N^{11} \\
&\quad + 155048N^{10} + 356978N^9 - 365210N^8 - 953263N^7 + 458455N^6 \\
&\quad + 924557N^5 - 305717N^4 - 358086N^3 - 66708N^2 + 87048N \\
&\quad + 38880.
\end{align*}\]
\[ \hat{A}^{(3),J_{1b}}_{Qg} = T_{F}^{2} n_{f} C_{A} \left\{ \frac{1}{N^{2}(N+1)^{2}} \left\{ -\frac{1}{\varepsilon^{3}} \left[ \frac{64(4N^{2} + 4N - 5)}{9} \right] \right. \right. \\
+ \frac{1}{\varepsilon^{2}} \left[ -\frac{32}{9} (4N^{2} + 4N - 5) S_{1} + \frac{32P_{41}(N)}{27N(N + 1)(N + 2)} \right] \\
+ \frac{1}{\varepsilon} \left[ -\frac{8}{9} (4N^{2} + 4N - 5) S_{1}^{2} - \frac{104}{9} (4N^{2} + 4N - 5) S_{2} \right] \\
\left. \left. - \frac{8}{3} (4N^{2} + 4N - 5) \zeta_{2} + \frac{16P_{41}(N)}{27N(N + 1)(N + 2)} \right] \right\} \right\}, \tag{D.52} \]

with

\[ P_{41}(N) = 44N^{5} + 191N^{4} + 99N^{3} - 17N^{2} + 136N + 60, \tag{D.53} \]
\[ P_{42}(N) = 232N^{8} + 1978N^{7} + 4292N^{6} + 4447N^{5} + 3446N^{4} - 1058N^{3} \\
- 5180N^{2} - 2712N - 720, \tag{D.54} \]
\[ P_{43}(N) = 1328N^{11} + 16796N^{10} + 66200N^{9} + 134952N^{8} + 148833N^{7} \\
+ 40020N^{6} - 52496N^{5} + 66940N^{4} + 180160N^{3} + 115296N^{2} \\
+ 45504N + 8640. \tag{D.55} \]
\[-8(N^3 - 10N^2 + 43N + 46)S_3 + \frac{28}{9}(N^3 - 10N^2 + 43N + 46)\zeta_3 \]
\[+ \frac{8P_{44}(N)}{9(N - 1)N(N + 1)(N + 2)}S_2 + \frac{2P_{44}(N)}{9(N - 1)N(N + 1)(N + 2)}\zeta_2 \]
\[+ \frac{4P_{46}(N)}{243(N - 1)^3N^3(N + 1)^3(N + 2)^3}, \]

(D.56)

with

\[P_{44}(N) = 11N^7 - 100N^6 + 317N^5 - 59N^4 - 2184N^3 - 765N^2 + 1064N + 276, \]

(D.57)

\[P_{45}(N) = 67N^{11} - 606N^{10} + 221N^9 - 5084N^8 - 7700N^7 + 41990N^6 + 48735N^5 - 45550N^4 - 33703N^3 + 18682N^2 + 7212N + 1656, \]

(D.58)

\[P_{46}(N) = 431N^{15} - 3320N^{14} - 7624N^{13} - 6288N^{12} + 161483N^{11} + 372478N^{10} - 690814N^9 - 1786393N^8 + 805264N^7 + 2328180N^6 - 851672N^5 - 1227601N^4 + 257348N^3 + 123792N^2 + 48240N + 9936. \]

(D.59)

\[
\hat{A}^{(3), K_{1b}}_{Qg} = \frac{T_F^2 n_f C_A}{(N - 1)N(N + 1)^2(N + 2)} \left\{ \frac{1}{\varepsilon^3} \left[ \frac{64(3N^2 - 23N - 20)}{9} \right] \right. \\
+ \frac{1}{\varepsilon^2} \left[ \frac{32(3N^2 - 23N - 20)}{9} S_1 \\
- \frac{32(54N^4 - 127N^3 - 289N^2 + 322N + 376)}{27(N + 1)(N + 2)} \right] \\
+ \frac{1}{\varepsilon} \left[ \frac{8(3N^2 - 23N - 20)}{9} S_2 + \frac{104(3N^2 - 23N - 20)}{9} S_2 \right. \\
+ \frac{8(3N^2 - 23N - 20)}{3} \zeta_2 \\
- \frac{16(54N^4 - 127N^3 - 289N^2 + 322N + 376)}{27(N + 1)(N + 2)} S_1 + \frac{16P_{47}(N)}{81(N + 1)^2(N + 2)^2} \right. \\
+ \frac{4(3N^2 - 23N - 20)}{27} S_1^3 \\
+ \frac{440(3N^2 - 23N - 20)}{27} S_3 - \frac{56(3N^2 - 23N - 20)}{9} \zeta_3 \\
+ \frac{52(3N^2 - 23N - 20)}{9} S_2 S_1 + \frac{4(3N^2 - 23N - 20)}{3} \zeta_2 S_1 \right. \\
\left. \right\} 
\]
\[
-\frac{4(54N^4 - 127N^3 - 289N^2 + 322N + 376)}{27(N+1)(N+2)} S_1^2 \\
-\frac{52(54N^4 - 127N^3 - 289N^2 + 322N + 376)}{27(N+1)(N+2)} S_2 \\
-\frac{4(54N^4 - 127N^3 - 289N^2 + 322N + 376)}{9(N+1)(N+2)} \zeta_2 \\
+ \frac{8P_{48}(N)}{81(N+1)^2(N+2)^2} S_1 \\
- \frac{8P_{49}(N)}{243(N+1)^3(N+2)^3} \right) ,
\]

(D.60)

with

\[
P_{47}(N) = 468N^6 + 574N^5 + 199N^4 + 1615N^3 - 5564N^2 - 18092N - 10304
\]

(D.61)

\[
P_{48}(N) = 468N^6 + 574N^5 + 199N^4 + 1615N^3 - 5564N^2 - 18092N - 10304
\]

(D.62)

\[
P_{49}(N) = 3096N^8 + 11084N^7 + 7658N^6 - 72687N^5 - 301881N^4 - 412434N^3 + 10260N^2 + 433240N + 231808
\]

(D.63)
\[ + \frac{29}{12} (4N + 5) S_2 - \frac{4N + 5}{2} \zeta_2 S_2 + \frac{17}{6} (4N + 5) S_4 + 4(4N + 5) S_{3,1} - 4(4N + 5) S_{2,1,1} - \frac{(260N^3 + 762N^2 + 451N - 12)}{81N(N + 1)} S_1^3 \]
\[ - \frac{(32N^3 + 96N^2 + 49N - 12)}{9N(N + 1)} \zeta_2 S_1 - \frac{14}{9} (4N + 5) \zeta_3 S_1 \]
\[ - \frac{(404N^3 + 834N^2 + 307N - 156)}{27N(N + 1)} S_2 S_1 - \frac{14(2N^3 + 5N^2 + 6N + 4)}{9N(N + 1)} \zeta_3 S_3 \]
\[ - \frac{2(908N^3 + 1086N^2 - 197N - 660)}{81N(N + 1)} S_3 - \frac{4(20N^2 + 90N + 61)}{9N(N + 1)} S_{2,1} \]
\[ + \frac{P_{53}(N)}{27N^2(N + 1)^2(N + 2)} S_1^2 - \frac{P_{50}(N)}{9N^2(N + 1)^2(N + 2)} \zeta_2 \]
\[ + \frac{P_{54}(N)}{27N^2(N + 1)^2(N + 2)} S_2 \]
\[ + \frac{P_{56}(N)}{486N^4(N + 1)^4(N + 2)^2} \right\}, \quad (D.64) \]

with

\[ P_{50}(N) = 43N^6 + 301N^5 + 587N^4 + 484N^3 + 132N^2 - 80N - 48 , \quad (D.65) \]
\[ P_{51}(N) = 190N^6 + 870N^5 + 802N^4 - 543N^3 - 938N^2 - 192N + 144 , \quad (D.66) \]
\[ P_{52}(N) = 991N^9 + 9415N^8 + 32215N^7 + 52113N^6 + 43252N^5 \]
\[ + 17484N^4 + 2928N^3 + 3104N^2 + 3648N + 1152 , \quad (D.67) \]
\[ P_{53}(N) = 276N^6 + 1472N^5 + 1976N^4 + 425N^3 - 674N^2 - 352N + 48 , \quad (D.68) \]
\[ P_{54}(N) = 948N^6 + 4328N^5 + 6176N^4 + 2945N^3 - 2N^2 + 608N + 624 , \quad (D.69) \]
\[ P_{55}(N) = 1379N^9 + 9765N^8 + 20193N^7 + 10203N^6 - 15291N^5 \]
\[ - 30216N^4 - 27620N^3 - 14160N^2 - 5472N - 1728 , \quad (D.70) \]
\[ P_{56}(N) = 21055N^{12} + 262474N^{11} + 1324746N^{10} + 3564860N^9 \]
\[ + 5666307N^8 + 5550126N^7 + 3387956N^6 + 1293128N^5 \]
\[ + 273984N^4 + 120320N^3 - 219648N^2 - 129024N - 27648 . \quad (D.71) \]
\[
\frac{1}{\varepsilon^2} \left\{ \frac{32}{27} S_1^2 + \frac{8}{3} \zeta_2 S_1 + \frac{64}{9} S_2 S_1 + \frac{208}{27} S_3 + \frac{64}{9} S_{2,1} - \frac{16(5N + 14)}{27(N + 1)} S_1^2 \\
+ \frac{2(2N^3 + 7N^2 + 6N + 3)}{3N(N + 1)^2} \zeta_2 - \frac{8(74N^3 + 121N^2 + 38N - 27)}{27N(N + 1)^2} S_2 \\
+ \frac{8(47N^3 + 13N^2 - 196N - 108)}{81N(N + 1)^2} S_1 + \frac{2P_{58}(N)}{81N^3(N + 1)^4(N + 2)^2} \right\}
\]

\[
+ \frac{8S_1^4}{27} - \frac{56}{9} \zeta_3 S_1 + \frac{4}{3} \zeta_2 S_1^2 + \frac{32}{9} S_2 S_1 + \frac{208}{27} S_3 S_1 + \frac{64}{9} S_{2,1} S_1 \\
+ \frac{80}{9} S_2^2 + \frac{8}{3} \zeta_2 S_2 + \frac{128}{9} S_4 + \frac{32}{3} S_{3,1} - \frac{64}{9} S_{2,1,1} \\
- \frac{16(5N + 14)}{81(N + 1)} S_1^3 - \frac{4(5N + 14)}{9(N + 1)} \zeta_2 S_1 \\
- \frac{32(5N + 14)}{27(N + 1)} S_2 S_1 - \frac{14(2N^3 + 7N^2 + 6N + 3)}{9N(N + 1)^2} \zeta_3 \\
- \frac{4(616N^3 + 899N^2 + 202N - 243)}{81N(N + 1)^2} S_3 - \frac{32(5N + 14)}{27(N + 1)} S_{2,1} \\
+ \frac{4(47N^3 + 13N^2 - 196N - 108)}{81N(N + 1)^2} S_1^2 - \frac{P_{57}(N)}{9N^2(N + 1)^3(N + 2)} \zeta_2 \\
+ \frac{4P_{59}(N)}{81N^2(N + 1)^3(N + 2)} S_2 - \frac{2P_{60}(N)}{243N^2(N + 1)^3} S_1 \\
- \frac{P_{61}(N)}{486N^4(N + 1)^5(N + 2)^3} \right\},
\] (D.72)

with

\[
P_{57}(N) = 43N^6 + 302N^5 + 566N^4 + 445N^3 + 129N^2 - 81N - 54, \] (D.73)
\[
P_{58}(N) = 1207N^9 + 11543N^8 + 40819N^7 + 70919N^6 + 65266N^5 + 27608N^4 + 312N^3 + 162N^2 + 3672N + 1512, \] (D.74)
\[
P_{59}(N) = 742N^6 + 3260N^5 + 5157N^4 + 3025N^3 + 251N^2 + 513N + 486, \] (D.75)
\[
P_{60}(N) = 323N^5 - 3972N^4 - 9291N^3 - 4456N^2 - 1080N + 648, \] (D.76)
\[
P_{61}(N) = 25807N^{12} + 324932N^{11} + 1659342N^{10} + 4520784N^9 + 7180599N^8 + 6692496N^7 + 3387488N^6 + 763528N^5 + 119892N^4 + 17388N^3 - 147960N^2 - 143856N - 38880. \] (D.77)
\[\begin{aligned}
&+ \frac{1}{\varepsilon} \left[ \frac{4}{9}(N^2 - 2N - 2)S_1^2 + \frac{4}{9}(5N - 14)(5N + 4)S_2 \\
&+ \frac{2}{3}(4N^2 - 8N - 9)\zeta_2 - \frac{8P_{63}(N)}{27N(N + 1)(N + 2)} S_1 \\
&- \frac{4P_{64}(N)}{81N^2(N + 1)^2(N + 2)} \right] + \frac{2}{27}(N^2 - 2N - 2)S_1^3 \\
&+ \frac{4}{27}(109N^2 - 218N - 245)S_3 - \frac{14}{9}(4N^2 - 8N - 9)\zeta_3 \\
&+ \frac{26}{9}(N^2 - 2N - 2)S_2 S_1 + \frac{2}{3}(N^2 - 2N - 2)\zeta_2 S_1 \\
&- \frac{2P_{63}(N)}{27N(N + 1)(N + 2)} S_1^2 + \frac{2P_{65}(N)}{27N(N + 1)(N + 2)} S_2 \\
&+ \frac{P_{66}(N)}{9N(N + 1)(N + 2)} \zeta_2 + \frac{4P_{66}(N)}{81N^2(N + 1)^2(N + 2)^2} S_1 \\
&+ \frac{2P_{67}(N)}{243N^3(N + 1)^3(N + 2)^3} \right]
\end{aligned}\]  
(D.78)

with

\[\begin{align*}
P_{62}(N) &= 12N^6 - 17N^5 - 155N^4 + 43N^3 + 83N^2 - 207N - 138, \\
P_{63}(N) &= 17N^5 + 59N^4 + 21N^3 - 38N^2 + 16N + 24, \\
P_{64}(N) &= 24N^8 - 91N^7 - 713N^6 - 558N^5 - 424N^4 - 1202N^3 + 912N^2 \\
&+ 205N + 918, \\
P_{65}(N) &= 72N^6 - 119N^5 - 989N^4 - 279N^3 + 536N^2 - 1258N - 852, \\
P_{66}(N) &= 88N^8 + 553N^7 + 977N^6 + 241N^5 - 436N^4 - 26N^3 - 296N^2 \\
&- 624N - 288, \\
P_{67}(N) &= 264N^6 + 1381N^5 - 4166N^4 + 47256N^3 - 152187N^2 \\
&- 251073N^7 - 189276N^6 + 16418N^5 + 68699N^4 - 79947N^3 \\
&- 148962N^2 - 95364N - 23112.
\end{align*}\]  
(D.79-84)

\[\begin{aligned}
A_{Q_9}^{(3), N_{1a}} &= \frac{T_f^2 n_f C_A}{N(N + 1)(N + 2)} \left\{ \frac{1}{\varepsilon^2} \left[ \frac{32}{9}(2N^2 + 3N + 2)S_1 \\
&- \frac{32(N^3 + 2N^2 + 1)}{9(N + 1)} \right] + \frac{1}{\varepsilon^2} \left[ \frac{8}{9}(6N^2 + 11N + 8)S_2 \\
&- \frac{64}{9}(N^2 - 4)S_{-2} - \frac{8}{9}(14N^2 + 33N + 12)S_2 \\
&- \frac{16P_{68}(N)}{27N(N + 1)(N + 2)} S_1 + \frac{16P_{69}(N)}{27N(N + 1)^2(N + 2)} \right]\right\}
\end{aligned}\]
\[\frac{1}{\varepsilon} \left[ \frac{4}{27} (14N^2 + 27N + 20)S_1^3 + \frac{4}{3} (2N^2 + 3N + 2)\zeta_2 S_1 \right.
\]
\[- \frac{32}{3} (N^2 - 4) S_{-2} S_1 - \frac{4}{9} (6N^2 + N - 44) S_2 S_1 \]
\[- \frac{80}{9} (N^2 - 4) S_{-3} + \frac{32}{3} (N^2 - 4) S_{-2,1} + \frac{16}{9} N(11N + 16) S_{2,1} \]
\[- \frac{8}{27} (94N^2 + 171N - 2) S_3 - \frac{4P_{70}(N)}{27N(N + 1)(N + 2)} S_1^2 - \frac{4(N^3 + 2N^2 + 1)}{3(N + 1)} \zeta_2 \]
\[+ \frac{64(7N^4 - 17N^3 - 43N^2 + 5N + 6)}{27N(N + 1)} S_{-2} + \frac{4P_{73}(N)}{27N(N + 1)(N + 2)} S_2 \]
\[+ \frac{8P_{71}(N)}{81N^3(N + 1)^2(N + 2)^2} S_1 - \frac{8P_{72}(N)}{81N^2(N + 1)^3(N + 2)^2} \]
\[+ \frac{1}{54} (30N^2 + 59N + 44) S_4^4 + \frac{1}{3} (6N^2 + 11N + 8) \zeta_2 S_1^2 \]
\[-8(N^2 - 4) S_{-2} S_2^2 + \frac{1}{9} (2N^2 + 63N + 188) S_2 S_1^2 \]
\[- \frac{28}{9} (2N^2 + 3N + 2) \zeta_3 S_1 - \frac{40}{3} (N^2 - 4) S_{-3} S_1 \]
\[- \frac{4}{27} (114N^2 + 67N - 368) S_3 S_1 + 16(N^2 - 4) S_{-2,1} S_1 \]
\[+ \frac{8}{9} (25N^2 + 32N - 12) S_{2,1} S_1 + \frac{1}{18} (6N^2 - 205N - 292) S_2^2 \]
\[+ \frac{8}{9} (N^2 - 4) S_{-4} - \frac{8}{3} (N^2 - 4) \zeta_2 S_{-2} \]
\[- \frac{1}{3} (14N^2 + 33N + 12) \zeta_2 S_2 - \frac{8}{3} (N^2 - 4) S_{-2} S_2 \]
\[- \frac{7}{9} (54N^2 + 99N - 4) S_1 + \frac{40}{3} (N^2 - 4) S_{-3,1} \]
\[- \frac{32}{3} (N^2 - 4) S_{2, -2} + \frac{16}{3} (7N^2 + 8N - 6) S_{3,1} \]
\[-16(N^2 - 4) S_{-2,1,1} - \frac{8}{9} (25N^2 + 32N - 12) S_{2,1,1} \]
\[- \frac{2P_{74}(N)}{81N(N + 1)(N + 2)} S_1^3 - \frac{2P_{68}(N)}{9N(N + 1)(N + 2)} \zeta_2 S_1 \]
\[+ \frac{32(7N^4 - 17N^3 - 43N^2 + 5N + 6)}{9N(N + 1)} S_{-2} S_1 + \frac{2P_{75}(N)}{27N(N + 1)(N + 2)} S_2 S_1 \]
\[+ \frac{28(N^3 + 2N^2 + 1)}{9(N + 1)} \zeta_3 + \frac{80(7N^4 - 17N^3 - 43N^2 + 5N + 6)}{27N(N + 1)} S_{-3} \]
\[+ \frac{4P_{76}(N)}{81N(N + 1)(N + 2)} S_3 + \frac{32(7N^4 - 17N^3 - 43N^2 + 5N + 6)}{9N(N + 1)} S_{-2,1} \]
\[+ \frac{16P_{77}(N)}{27N(N + 1)(N + 2)} S_{2,1} + \frac{2P_{78}(N)}{81N^2(N + 1)^2(N + 2)^2} S_1^2 \]
\[+ \frac{2P_{69}(N)}{9N(N + 1)^2(N + 2)} \zeta_2 - \frac{32P_{70}(N)}{81N^2(N + 1)^2(N + 2)} S_{-2} \]
$$-\frac{2P_{80}(N)}{81N^2(N+1)^2(N+2)^2} S_2 - \frac{4P_{81}(N)}{243N^3(N+1)^3(N+2)^3} S_1 + \frac{4P_{82}(N)}{243N^3(N+1)^4(N+2)^3}$$

with

$$P_{68}(N) = 16N^5 + 72N^4 + 75N^3 - 138N^2 - 232N - 48,$$  \hspace{1cm} (D.86)

$$P_{69}(N) = 14N^6 + 67N^5 + 85N^4 + 37N^3 - 18N^2 - 47N - 6,$$  \hspace{1cm} (D.87)

$$P_{70}(N) = 42N^5 + 217N^4 + 316N^3 - 190N^2 - 532N - 144,$$  \hspace{1cm} (D.88)

$$P_{71}(N) = 140N^8 + 1131N^7 + 2545N^6 - 258N^5 - 6077N^4 - 4596N^3$$
$$+ 476N^2 + 816N + 288,$$  \hspace{1cm} (D.89)

$$P_{72}(N) = 154N^9 + 1208N^8 + 3481N^7 + 4866N^6 + 3091N^5 + 612N^4$$
$$+ 975N^3 + 1549N^2 + 336N + 36,$$  \hspace{1cm} (D.90)

$$P_{73}(N) = 82N^5 + 417N^4 + 686N^3 + 210N^2 - 348N - 144,$$  \hspace{1cm} (D.91)

$$P_{74}(N) = 94N^5 + 507N^4 + 798N^3 - 294N^2 - 1132N - 336,$$  \hspace{1cm} (D.92)

$$P_{75}(N) = 90N^5 - 283N^4 - 1618N^3 - 410N^2 + 1900N + 432,$$  \hspace{1cm} (D.93)

$$P_{76}(N) = 716N^5 + 2238N^4 + 939N^3 - 2532N^2 - 2252N - 528,$$  \hspace{1cm} (D.94)

$$P_{77}(N) = 47N^5 + 136N^4 + 10N^3 - 295N^2 - 252N - 60,$$  \hspace{1cm} (D.95)

$$P_{78}(N) = 336N^8 + 2909N^7 + 7295N^6 + 2096N^5 - 11749N^4 - 9748N^3$$
$$+ 1580N^2 + 2448N + 864,$$  \hspace{1cm} (D.96)

$$P_{79}(N) = 50N^7 - N^6 - 70N^5 + 530N^4 + 716N^3 - 97N^2 - 84N - 36,$$  \hspace{1cm} (D.97)

$$P_{80}(N) = 344N^8 + 2775N^7 + 9197N^6 + 13188N^5 + 6341N^4 + 1560N^3$$
$$+ 4404N^2 + 2880N + 864,$$  \hspace{1cm} (D.98)

$$P_{81}(N) = 1252N^{11} + 14118N^{10} + 58795N^9 + 122580N^8 + 153807N^7$$
$$+ 131190N^6 + 43487N^5 - 64116N^4 - 66172N^3 - 14880N^2$$
$$- 7488N - 1728,$$  \hspace{1cm} (D.99)

$$P_{82}(N) = 1550N^{12} + 16786N^{11} + 74226N^{10} + 174527N^9 + 224721N^8$$
$$+ 133572N^7 - 9824N^6 - 69685N^5 - 68916N^4 - 46499N^3$$
$$- 12426N^2 - 2340N - 216.$$  \hspace{1cm} (D.100)

$$\zeta^{(3),N_{16}}_{Q_{9g}} = \frac{T_{f}^{2} n_{f} C_{A}}{N(N+1)(N+2)} \left\{ \frac{1}{\varepsilon^{3}} \left[ \frac{16}{9}(4N^2 + 5N + 2)S_1 \right]\right.$$
$$- \frac{32N(N^2 + 2N - 2)}{9(N+1)} \varepsilon + \frac{1}{\varepsilon^{2}} \left[ \frac{4}{9}(8N^2 + 5N - 2)S_2 \right] - \frac{128}{9}(N - 1)(N + 2)S_{-2}$$
$$- \frac{4}{9}(32N^2 + 71N + 18)S_2 - \frac{8P_{83}(N)}{27N(N+1)(N+2)} S_1 + \frac{16P_{84}(N)}{27(N+1)^2(N+2)} \right\}$$
\[
\frac{1}{\epsilon}\left[\frac{2}{27}(16N^2 + 5N - 10)S_1^3 + \frac{2}{3}(4N^2 + 5N + 2)\zeta_2 S_1 \right. \\
- \frac{256}{9}(N - 1)(N + 2)S_{-2}S_1 - \frac{2}{9}(48N^2 + 59N - 118)S_2S_1 \\
- \frac{160}{9}(N - 1)(N + 2)S_{-3} + \frac{64}{3}(N - 1)(N + 2)S_{-2,1} \\
+ \frac{8}{9}(28N^2 + 31N - 26)S_{2,1} - \frac{4}{27}(284N^2 + 457N - 158)S_3 \\
- \frac{2P_{55}(N)}{27N(N + 1)(N + 2)}S_1^2 - \frac{4N(N^2 + 2N - 2)}{3(N + 1)}\zeta_2 \\
+ \frac{64(11N^3 - 14N^2 - 59N - 10)}{27(N + 1)}S_{-2} + \frac{2P_{56}(N)}{27N(N + 1)(N + 2)}S_2 \\
+ \frac{4P_{87}(N)}{81N(N + 1)^2(N + 2)^2}S_1 - \left. \frac{8P_{88}(N)}{81(N + 1)^3(N + 2)^2} \right]
\]

\[
\frac{1}{108}(32N^2 + 5N - 26)S_1^4 + \frac{1}{6}(8N^2 + 5N - 2)\zeta_2 S_1^2 \\
- \frac{256}{9}(N - 1)(N + 2)S_{-2}S_1^2 + \frac{1}{18}(-224N^2 - 251N + 486)S_2S_1^2 \\
- \frac{14}{9}(4N^2 + 5N + 2)\zeta_3 S_1 - \frac{320}{9}(N - 1)(N + 2)S_{-3}S_1 \\
- \frac{2}{27}(736N^2 + 763N - 1510)S_3S_1 + \frac{128}{3}(N - 1)(N + 2)S_{-2,1}S_1 \\
+ \frac{4}{9}(88N^2 + 79N - 134)S_{2,1}S_1 + \frac{1}{36}(128N^2 - 403N - 1034)S_2^2 \\
+ \frac{16}{9}(N - 1)(N + 2)S_{-4} - \frac{16}{3}(N - 1)(N + 2)\zeta_2 S_{-2} \\
+ \frac{1}{6}(-32N^2 - 71N - 18)\zeta_2 S_2 - \frac{64}{9}(N - 1)(N + 2)S_{-2}S_2 \\
- \frac{64}{3}(N - 1)(N + 2)S_{-2,2} + \frac{1}{18}(-1120N^2 - 1903N + 526)S_4 \\
+ \frac{80}{3}(N - 1)(N + 2)S_{-3,1} + \frac{4}{3}(48N^2 + 45N - 82)S_{3,1} \\
- 32(N - 1)(N + 2)S_{-2,1,1} - \frac{4}{9}(68N^2 + 41N - 142)S_{2,1,1} \\
- \frac{P_{89}(N)}{81N(N + 1)(N + 2)}S_1^3 - \frac{P_{83}(N)}{9N(N + 1)(N + 2)}\zeta_2 S_1 \\
+ \frac{128(11N^3 - 14N^2 - 59N - 10)}{27(N + 1)}S_{-2}S_1 + \frac{P_{90}(N)}{27N(N + 1)(N + 2)}S_2S_1 \\
+ \frac{28N(N^2 + 2N - 2)}{9(N + 1)}\zeta_3 + \frac{2P_{91}(N)}{81N(N + 1)(N + 2)}S_3 \\
+ \frac{80(11N^3 - 14N^2 - 59N - 10)}{27(N + 1)}S_{-3} - \frac{4P_{92}(N)}{27N(N + 1)(N + 2)}S_{2,1} \\
+ \frac{32(11N^3 - 14N^2 - 59N - 10)}{9(N + 1)}S_{-2,1} + \frac{P_{93}(N)}{81N(N + 1)^2(N + 2)^2}S_1^2
\]
\[
\frac{2P_{84}(N)}{9(N+1)^2(N+2)}\zeta_2 - \frac{128P_{94}(N)}{81(N+1)^2(N+2)}S_{-2}
\]
\[
- \frac{P_{95}(N)}{81N(N+1)^2(N+2)^2}S_2 - \frac{2P_{96}(N)}{243N(N+1)^3(N+2)^3}S_1
\]
\[
+ \frac{4P_{97}(N)}{243(N+1)^4(N+2)^3} \right) ,
\]

with

\[
P_{83}(N) = 20N^5 + 76N^4 + 35N^3 - 256N^2 - 316N - 96 , \quad (D.102)
\]
\[
P_{84}(N) = 8N^5 + 43N^4 + 45N^3 + 29N^2 + 22N - 24 , \quad (D.103)
\]
\[
P_{85}(N) = 40N^5 + 94N^4 - 155N^3 - 856N^2 - 836N - 192 , \quad (D.104)
\]
\[
P_{86}(N) = 184N^5 + 622N^4 + 251N^3 - 1240N^2 - 1596N - 384 , \quad (D.105)
\]
\[
P_{87}(N) = 184N^7 + 1388N^6 + 2586N^5 - 2671N^4 - 12540N^3
\]
\[
- 13444N^2 - 6160N - 960 , \quad (D.106)
\]
\[
P_{88}(N) = 88N^7 + 530N^6 + 227N^5 - 3946N^4 - 11473N^3 - 14065N^2
\]
\[
- 7202N - 528 , \quad (D.107)
\]
\[
P_{89}(N) = 80N^5 + 130N^4 - 535N^3 - 2056N^2 - 1876N - 384 , \quad (D.108)
\]
\[
P_{90}(N) = 624N^5 + 454N^4 - 4961N^3 - 7000N^2 - 844N + 384 , \quad (D.109)
\]
\[
P_{91}(N) = 2248N^5 + 4052N^4 - 9473N^3 - 22736N^2 - 11468N - 2208 , \quad (D.110)
\]
\[
P_{92}(N) = 236N^5 + 374N^4 - 1269N^3 - 3032N^2 - 1628N - 288 , \quad (D.111)
\]
\[
P_{93}(N) = 368N^7 + 2498N^6 + 3042N^5 - 12661N^4 - 37056N^3
\]
\[
- 35356N^2 - 14144N - 1920 , \quad (D.112)
\]
\[
P_{94}(N) = 19N^5 + 23N^4 + N^3 + 131N^2 + 178N - 28 , \quad (D.113)
\]
\[
P_{95}(N) = 1376N^7 + 7298N^6 + 11630N^5 - 8683N^4 - 47392N^3
\]
\[
- 46660N^2 - 15168N - 3840 , \quad (D.114)
\]
\[
P_{96}(N) = 1448N^9 + 14464N^8 + 45664N^7 + 27660N^6 - 157311N^5
\]
\[
- 465972N^4 - 638594N^3 - 483184N^2 - 176200N - 21120 , \quad (D.115)
\]
\[
P_{97}(N) = 824N^9 + 7474N^8 + 20726N^7 - 2277N^6 - 140187N^5
\]
\[
- 335448N^4 - 349868N^3 - 155743N^2 - 25874N - 11616 . \quad (D.116)
\]

\[
\tilde{\zeta}^{(3,O_1)}_{A_{Qg}} = \frac{T^2_{P>n}C_A}{(N+1)(N+2)} \left\{ \frac{1}{\varepsilon^3} \left[ -\frac{16(9N+10)}{9N}S_1 - \frac{128(2N+3)}{9(N+1)(N+2)} \right] \right.
\]
\[
+ \frac{1}{\varepsilon^2} \left[ -\frac{4(23N+26)}{9N}S_2 - \frac{4(31N+34)}{9N}S_1 \right]
\]
\[
+ \frac{8(96N^3 + 383N^2 + 552N + 268)}{27N(N+1)(N+2)}S_1
\]
\[
+ \frac{16(99N^4 + 562N^3 + 1035N^2 + 656N + 48)}{27(N+1)^2(N+2)^2} \right\} + \frac{1}{\varepsilon} \left[ -\frac{2(51N+58)}{27N}S_1 \right]
\]
\[
\begin{align*}
&\frac{2(9N + 10)}{3N} \zeta_2 S_1 - \frac{2(67N + 74)}{9N} S_2 S_1 - \frac{4(87N + 94)}{27N} S_3 \\
&- \frac{8(23N + 26)}{9N} S_{2,1} - \frac{16(2N + 3)}{3(N + 1)(N + 2)} \zeta_2 \\
&+ \frac{2(644N^3 + 2135N^2 + 2692N + 1516)}{27N(N + 1)(N + 2)} S_2 \\
&+ \frac{2(244N^3 + 1003N^2 + 1436N + 668)}{27N(N + 1)(N + 2)} S_1^2 + \frac{4P_{102}(N)}{81N(N + 1)^2(N + 2)^2} S_1 \\
&- \frac{4P_{103}(N)}{81(N + 1)^3(N + 2)^3} \left(\frac{107N + 122}{108N}\right) S_1^4 \\
&+ \frac{(540N^3 + 2243N^2 + 3204N + 1468)}{81N(N + 1)(N + 2)} S_1^3 - \frac{4(23N + 26)}{3N} S_{3,1} \\
&+ \frac{4(61N + 70)}{9N} S_{2,1,1} - \frac{(139N + 154)}{31N + 34} \zeta_2 S_2 S_1^2 - \frac{23N + 26}{6N} \zeta_2 S_1^2 \\
&- \frac{2(179N + 194)}{27N} S_3 S_1 - \frac{4(61N + 70)}{9N} S_{2,1} S_1 + \frac{14(9N + 10)}{9N} \zeta_3 S_1 \\
&- \frac{(511N + 562)}{18N} S_4 + \frac{2(2340N^3 + 7337N^2 + 8856N + 5284)}{81N(N + 1)(N + 2)} S_3 \\
&+ \frac{836N^3 + 3283N^2 + 4636N + 2300}{27N(N + 1)(N + 2)} S_2 S_1 + \frac{112(2N + 3)}{9(N + 1)(N + 2)} \zeta_3 \\
&+ \frac{4(214N^3 + 889N^2 + 1298N + 596)}{27N(N + 1)(N + 2)} S_{2,1} \\
&+ \frac{(96N^3 + 383N^2 + 552N + 268)}{9N(N + 1)(N + 2)} \zeta_2 S_1 - \frac{P_{98}(N)}{81N(N + 1)^2(N + 2)^2} S_1^2 \\
&- \frac{P_{101}(N)}{81N(N + 1)^2(N + 2)^2} S_2 \\
&+ \frac{2(99N^4 + 562N^3 + 1035N^2 + 656N + 48)}{9(N + 1)^2(N + 2)^2} \zeta_2 \\
&- \frac{2P_{99}(N)}{243N(N + 1)^3(N + 2)^3} S_1 + \frac{P_{100}(N)}{243(N + 1)^4(N + 2)^4} \right) , \tag{D.117}
\end{align*}
\]

with

\[
\begin{align*}
P_{98}(N) &= 560N^5 + 4964N^4 + 24041N^3 + 55706N^2 + 58136N + 22256 , \tag{D.118} \\
P_{99}(N) &= 5646N^7 + 27934N^6 - 28488N^5 - 426969N^4 - 6094262N^3 \\
&- 1202880N^2 - 648456N - 133672 , \tag{D.119} \\
P_{100}(N) &= 6646N^8 + 706420N^7 + 3202098N^6 + 8134152N^5 \\
&+ 12726405N^4 + 12559980N^3 + 7477056N^2 + 2214080N \\
&+ 120576 , \tag{D.120} \\
P_{101}(N) &= 4996N^5 + 40516N^4 + 140065N^3 + 238954N^2 + 191872N \\
&+ 54736 , \tag{D.121} 
\end{align*}
\]
\[ P_{102}(N) = 42N^5 - 388N^4 - 6171N^3 - 18898N^2 - 21564N - 8416, \quad (D.122) \]

\[ P_{103}(N) = 2745N^6 + 20977N^5 + 59601N^4 + 76519N^3 + 40266N^2 + 3700N - 480. \quad (D.123) \]
\[ p_{104}(N) = 38N^5 + 1660N^4 + 6647N^3 + 10051N^2 + 7013N + 2464 , \quad (D.125) \]
\[ p_{105}(N) = 307N^5 + 2794N^4 + 9631N^3 + 16150N^2 + 13219N + 4240 , \quad (D.126) \]
\[ p_{106}(N) = 24N^5 - 3140N^4 - 13401N^3 - 20075N^2 - 13587N - 4928 , \quad (D.127) \]
\[ p_{107}(N) = 1052N^5 + 8260N^4 + 25625N^3 + 40447N^2 + 32003N + 9856 , \quad (D.128) \]
\[ p_{108}(N) = 1210N^7 + 22502N^6 + 119904N^5 + 319074N^4 + 502572N^3 + 486540N^2 + 259511N + 49600 , \quad (D.129) \]
\[ p_{109}(N) = 3395N^7 + 40451N^6 + 201441N^5 + 547869N^4 + 879225N^3 + 832767N^2 + 431665N + 94720 . \quad (D.130) \]
\[ \begin{align*}
&+ \frac{2(20N^3 - 1475N^2 - 3278N - 1204)}{27(N+1)(N+2)} S_2 S_1 + \frac{56(2N^2 + 7N + 2)}{9(N+2)} \zeta_3 \\
&- \frac{4(574N^3 + 1475N^2 + 1550N + 1852)}{81(N+1)(N+2)} S_3 + \frac{8(2N^3 - 257N^2 - 542N - 172)}{9(N+1)(N+2)} S_{2,1} \\
&+ \frac{2P_{113}(N)}{81(N+1)^2(N+2)^2} S_1^2 + \frac{4P_{110}(N)}{9(N+1)(N+2)^2} S_2 + \frac{2P_{114}(N)}{81(N+1)^2(N+2)^2} S_2 \\
&- \frac{4P_{115}(N)}{243(N+1)^3(N+2)^3} S_1 + \frac{8P_{116}(N)}{243N^3(N+1)^3(N+2)^4} \right\} ,
\end{align*} \]

(D.131)

with

\[ \begin{align*}
P_{110}(N) &= 22N^5 + 134N^4 + 204N^3 + 25N^2 - 88N - 12 , \\
P_{111}(N) &= 140N^5 + 3958N^4 + 15101N^3 + 22156N^2 + 15566N + 6088 , \\
P_{112}(N) &= 458N^8 + 4306N^7 + 15574N^6 + 28027N^5 + 26233N^4 \\
&\quad + 12193N^3 + 2798N^2 + 636N + 72 , \\
P_{113}(N) &= 290N^5 + 9918N^4 + 39839N^3 + 62088N^2 + 46622N \\
&\quad + 18264 , \\
P_{114}(N) &= 1094N^6 + 9414N^5 + 31391N^4 + 52296N^3 + 41630N^2 \\
&\quad + 11064N - 864 , \\
P_{115}(N) &= 4276N^7 + 68264N^6 + 351618N^5 + 915849N^4 + 1394436N^3 \\
&\quad + 1270848N^2 + 610766N + 89584 , \\
P_{116}(N) &= 4426N^{11} + 52400N^{10} + 256348N^9 + 673350N^8 + 1012896N^7 \\
&\quad + 836430N^6 + 281102N^5 - 71327N^4 - 82696N^3 - 22728N^2 \\
&\quad - 4464N - 432 .
\end{align*} \]

(D.132) - (D.138)

\[ \hat{A}_{Qg}^{(3),Q_1} = 0 . \]  \hspace{1cm} (D.139)

\[ \hat{A}_{Qg}^{(3),R_1} = 0 . \]  \hspace{1cm} (D.140)

\[ \hat{A}_{Qg}^{(3),R_1^*} = 0 . \]  \hspace{1cm} (D.141)

\[ \hat{A}_{Qg}^{(3),R_1^b} = 0 . \]  \hspace{1cm} (D.142)
\[
\hat{A}_{Qg}^{(3),S_{1b}} = \frac{T_F^2 n_f C_A}{N^2(N+1)^2} \left\{ \frac{1}{\varepsilon^3} \left[ \frac{16(N + 2)}{9} \right] \right. \\
+ \frac{1}{\varepsilon^2} \left[ \frac{8}{9}(N + 2)S_1 + \frac{8(32N^4 + 73N^3 + 10N^2 - 64N - 24)}{27N(N + 1)(N + 2)} \right] \\
+ \frac{1}{\varepsilon} \left[ -\frac{2}{9}(N + 2)S_1^2 - \frac{26}{9}(N + 2)S_2 - \frac{2}{3}(N + 2)\zeta_2 \right] \\
+ \frac{4(32N^4 + 73N^3 + 10N^2 - 64N - 24)}{27N(N + 1)(N + 2)} S_1 \\
- \frac{4P_{117}(N)}{81N^2(N + 1)^2(N + 2)^2} - \frac{1}{27}(N + 2)S_1^3 - \frac{110}{27}(N + 2)S_3 \\
+ \frac{14}{9}(N + 2)\zeta_3 - \frac{13}{9}(N + 2)S_2 S_1 - \frac{1}{3}(N + 2)\zeta_2 S_1 \\
+ \frac{1(32N^4 + 73N^3 + 10N^2 - 64N - 24)}{27N(N + 1)(N + 2)} S_1^2 \\
+ \frac{13(32N^4 + 73N^3 + 10N^2 - 64N - 24)}{27N(N + 1)(N + 2)} S_2 \\
+ \frac{(32N^4 + 73N^3 + 10N^2 - 64N - 24)}{9N(N + 1)(N + 2)} \zeta_2 \\
- \frac{2P_{117}(N)}{81N^2(N + 1)^2(N + 2)^2} S_1 + \frac{2P_{118}(N)}{243N^3(N + 1)^3(N + 2)^3} \right\} , \quad (D.143)
\]

with

\[
P_{117}(N) = 352N^7 + 1166N^6 + 775N^5 - 550N^4 + 436N^3 + 1976N^2 + 1200N + 288 , \quad (D.144)
\]

\[
P_{118}(N) = 2432N^{10} + 12004N^9 + 24210N^8 + 36105N^7 + 56184N^6 + 49188N^5 - 15320N^4 - 62080N^3 - 47040N^2 - 19584N - 3456 . \quad (D.145)
\]
\[ + \frac{4(4N^4 + 43N^3 + 26N^2 - 64N - 24)}{27(N(N + 1)(N + 2)} S_1 - \frac{4P_{119}(N)}{81N^2(N + 1)^2(N + 2)^2} \]
\[ + \frac{1}{27}(N - 2)S_3^3 + \frac{110}{27}(N - 2)S_3 - \frac{14}{9}(N - 2)\zeta_3 + \frac{13}{9}(N - 2)S_2S_1 \]
\[ + \frac{1}{3}(N - 2)\zeta_2S_1 + \frac{(4N^4 + 43N^3 + 26N^2 - 64N - 24)}{27N(N + 1)(N + 2)} S_1^2 \]
\[ + \frac{13(4N^4 + 43N^3 + 26N^2 - 64N - 24)}{9N(N + 1)(N + 2)} \zeta_2 \]
\[ - \frac{2P_{119}(N)}{81N^2(N + 1)^2(N + 2)^2} S_1 + \frac{2P_{120}(N)}{243N^3(N + 1)^3(N + 2)^3} \]  

with

\[ P_{119}(N) = 152N^7 + 722N^6 + 461N^5 - 1186N^4 - 364N^3 + 1976N^2 + 1200N + 288 \]  
\[ P_{120}(N) = 1168N^{10} + 6028N^9 + 8238N^8 + 5523N^7 + 27480N^6 + 51132N^5 - 1240N^4 - 62080N^3 - 47040N^2 + 19584N - 3456 \]

\[ A_{Q_9}^{(3),\tau_{1a}} = \frac{T_F^2n_fC_A}{(N - 1)N(N + 2)} \left\{ \frac{1}{\varepsilon^3} + \frac{1}{\varepsilon^2} \left[ \frac{32}{9} S_1 \right. \right. \]
\[ - \frac{64(7N^2 + 6N - 10)}{27(N + 1)(N + 2)} S_1 \]
\[ - \frac{32(7N^2 + 6N - 10)}{27(N + 1)(N + 2)} S_1 \]
\[ + \frac{64(25N^4 + 45N^3 - 14N^2 + 36N + 124)}{81(N + 1)^2(N + 2)^2} S_1 \]
\[ - \frac{56}{9} \zeta_3 + \frac{52}{9} S_2S_1 + \frac{4}{3} \zeta_2S_1 - \frac{8(7N^2 + 6N - 10)}{27(N + 1)(N + 2)} S_1^2 \]
\[ - \frac{104(7N^2 + 6N - 10)}{27(N + 1)(N + 2)} S_2 - \frac{8(7N^2 + 6N - 10)}{9(N + 1)(N + 2)} \zeta_2 \]
\[ + \frac{32(25N^4 + 45N^3 - 14N^2 + 36N + 124)}{81(N + 1)^2(N + 2)^2} S_1 \]
\[ - \frac{64P_{121}(N)}{243(N + 1)^3(N + 2)^3} \left\} \right\}, \]  

with

\[ P_{121}(N) = 79N^6 + 336N^5 + 765N^4 + 1488N^3 + 1392N^2 - 744N - 1480 \]
\[
\tilde{\chi}^{(3),T_{1b}}_{Qg} = \frac{T^2_{\bar{F}n_fC_A}}{(N - 1)N(N + 1)^2(N + 2)} \left\{ \frac{1}{\varepsilon^3} \left[ \frac{64(N + 3)}{9} \right] \right. \\
+ \frac{1}{\varepsilon^2} \left[ \frac{32}{9}(N + 3)S_1 - \frac{32(11N^3 + 39N^2 + 10N - 36)}{27(N + 1)(N + 2)} \right] \\
+ \frac{1}{\varepsilon} \left[ \frac{8}{9}(N + 3)S_1^2 + \frac{104}{9}(N + 3)S_2 + \frac{8}{3}(N + 3)\zeta_2 \right. \\
- \frac{16(11N^3 + 39N^2 + 10N - 36)}{27(N + 1)(N + 2)} S_1 + \frac{16P_{122}(N)}{81(N + 1)^2(N + 2)^2} \\
+ \frac{4}{27}(N + 3)S_1^3 + \frac{440}{27}(N + 3)S_3 - \frac{56}{9}(N + 3)\zeta_3 \\
+ \frac{52}{9}(N + 3)S_2S_1 + \frac{4}{3}(N + 3)\zeta_2 S_1 - \frac{4(11N^3 + 39N^2 + 10N - 36)}{27(N + 1)(N + 2)} S_1^2 \\
- \frac{52(11N^3 + 39N^2 + 10N - 36)}{27(N + 1)(N + 2)} S_2 - \frac{4(11N^3 + 39N^2 + 10N - 36)}{9(N + 1)(N + 2)} \zeta_2 \\
+ \frac{8P_{122}(N)}{81(N + 1)^2(N + 2)^2} S_1 - \frac{8P_{123}(N)}{243(N + 1)^3(N + 2)} \} , \quad (D.151)
\]

with

\[
P_{122}(N) = 58N^5 + 225N^4 + 181N^3 + 324N^2 + 1372N + 1296 , \quad (D.152)
\]
\[
P_{123}(N) = 332N^7 + 2418N^6 + 9531N^5 + 27393N^4 + 45426N^3 + 24108N^2 - 24536N - 25920 . \quad (D.153)
\]
\[ \begin{align*}
+ \frac{26}{9} (N^2 + 3N + 4)S_2S_1 + \frac{2}{3} (N^2 + 3N + 4)\zeta_2S_1 \\
- \frac{2(14N^4 + 51N^3 + 57N^2 - 18N - 56)}{27(N + 1)(N + 2)}S_2 \\
- \frac{26(14N^4 + 51N^3 + 57N^2 - 18N - 56)}{27(N + 1)(N + 2)}\zeta_2 \\
- \frac{4P_{124}(N)}{81(N + 1)^2(N + 2)^2}S_1
\end{align*} \] (D.154)

with

\[ P_{124}(N) = 100N^6 + 438N^5 + 629N^4 + 393N^3 + 1052N^2 + 2508N + 1792, \] (D.155)

\[ P_{125}(N) = 632N^8 + 4284N^7 + 14546N^6 + 36363N^5 + 68457N^4 + 73650N^3 + 11500N^2 - 54168N - 37760. \] (D.156)

\[ \hat{A}_{Qg}^{(3),A_2} = \frac{T_{\bar{f}f}^2 C_F}{(N - 1)N^2(N + 1)(N + 2)} \left\{ -\frac{1}{3} \frac{1512}{\varepsilon^3} \right\} \\
+ \frac{1}{\varepsilon} \left[ -\frac{128(3N^4 - 14N^3 - 21N^2 + 16N + 4)}{3(N - 1)N(N + 1)(N + 2)} \right] \\
+ \frac{1}{\varepsilon} \left[ -256S_2 - 64\zeta_2 + \frac{64P_{126}(N)}{3(N - 1)^2N^2(N + 1)^2(N + 2)^2} \right] \\
- 384S_3 + \frac{448}{3}\zeta_3 + \frac{64(3N^4 - 14N^3 - 21N^2 + 16N + 4)}{(N - 1)N(N + 1)(N + 2)}S_2 \\
+ \frac{16(3N^4 - 14N^3 - 21N^2 + 16N + 4)}{(N - 1)N(N + 1)(N + 2)}\zeta_2 \\
+ \frac{32P_{127}(N)}{3(N - 1)^3N^3(N + 1)^3(N + 2)^3} \right\}, \] (D.157)

with

\[ P_{126}(N) = N^8 + 34N^7 - 45N^6 - 239N^5 + 38N^4 + 269N^3 - 86N^2 - 36N - 8, \] (D.158)

\[ P_{127}(N) = 4N^{12} + 34N^{11} + 286N^{10} - 20N^9 - 1845N^8 - 826N^7 + 3276N^6 + 632N^5 - 2657N^4 + 396N^3 + 192N^2 + 80N + 16. \] (D.159)
$$\hat{A}_{Qg}^{(3), B_2} = \frac{T_F^2 n_f C_F}{N^3 (N + 1)^2} \left\{ -\frac{1}{\varepsilon^3} \left[ \frac{64(N - 1)(N + 2)}{3} \right] + \frac{1}{\varepsilon^2} \left[ \frac{32 P_{128}(N)}{3(N - 1) N (N + 1)(N + 2)} \right] \right. \\
+ \frac{1}{\varepsilon} \left[ -32(N - 1)(N + 2) S_2 - 8(N - 1)(N + 2) \zeta_2 - \frac{16 P_{129}(N)}{3(N - 1)^2 N^2 (N + 1)^2 (N + 2)^2} \right] - 48(N - 1)(N + 2) S_3 + \frac{56}{3} (N - 1)(N + 2) \zeta_3 + \frac{16 P_{128}(N)}{(N - 1) N (N + 1)(N + 2)} S_2 \\
+ \frac{4 P_{128}(N)}{(N - 1) N (N + 1)(N + 2)} \zeta_2 + \frac{8 P_{130}(N)}{3(N - 1)^3 N^3 (N + 1)^3 (N + 2)^3} \right\}, \quad (D.160)$$

with

$$P_{128}(N) = 2N^6 + 4N^5 - 13N^4 + 14N^3 + 41N^2 - 12N - 12, \quad (D.161)$$

$$P_{129}(N) = N^{10} + N^9 - 13N^8 + 100N^7 + 46N^6 - 494N^5 - 212N^4 + 473N^3 + 110N^2 - 100N - 56, \quad (D.162)$$

$$P_{130}(N) = 4N^{14} + 26N^{13} + 67N^{12} + 134N^{11} - 719N^{10} - 1462N^9 + 3010N^8 + 5074N^7 - 4187N^6 - 5412N^5 + 2609N^4 + 2240N^3 + 296N^2 - 576N - 240. \quad (D.163)$$

$$\hat{A}_{Qg}^{(3), C_2} = T_F^2 n_f \left( C_F - \frac{C_A}{2} \right) \frac{1}{(N-1)N(N+1)^2(N+2)^2} \left\{ \frac{1}{\varepsilon^3} \left[ \frac{2048}{3} \right] + \frac{1}{\varepsilon^2} \left[ -\frac{256 P_{131}(N)}{3(N - 1) N (N + 1)(N + 2)} \right] \right. \\
+ \frac{1}{\varepsilon} \left[ 1024S_2 + 256\zeta_2 + \frac{128 P_{132}(N)}{3(N - 1)^2 N^2 (N + 1)^2 (N + 2)^2} \right] \\
+ 1536S_3 - \frac{1792\zeta_3}{3} - \frac{128 P_{131}(N)}{(N - 1) N (N + 1)(N + 2)} S_2 \\
- \frac{32 P_{131}(N)}{(N - 1) N (N + 1)(N + 2)} \zeta_2 + \frac{64 P_{133}(N)}{3(N - 1)^3 N^3 (N + 1)^3 (N + 2)^3} \right\}, \quad (D.164)$$
with

\[ P_{131}(N) = N^5 + 9N^4 - 25N^3 - 53N^2 - 4 , \quad \text{(D.165)} \]
\[ P_{132}(N) = 3N^9 + 5N^8 - 71N^7 + 66N^6 + 531N^5 + 243N^4 - 267N^3 + 14N^2 - 84N - 8 , \quad \text{(D.166)} \]
\[ P_{133}(N) = 4N^{13} + 10N^{12} + 38N^{11} + 568N^{10} + 201N^9 - 3687N^8 - 3872N^7 + 3330N^6 + 2677N^5 - 1573N^4 + 648N^3 - 744N^2 - 176N - 16 . \quad \text{(D.167)} \]

\[ \hat{A}_{Qg}^{(3),D2} = T_F^2 n_f \left( C_F - \frac{C_A}{2} \right) \frac{1}{N^2(N+1)^3} \left\{ \frac{1}{\varepsilon^3} \frac{1256(N-1)}{3} - \frac{1}{\varepsilon^2} \left[ \frac{128P_{134}(N)}{3N(N+1)(N+2)^2(N-1)} \right] + \frac{1}{\varepsilon} \left[ 128(N-1)S_2 \right] + 32(N-1)\zeta_2 \right. \]
\[ + \left. \frac{32P_{135}(N)}{3(N-1)^2N^2(N+1)^2(N+2)^3} \right) + 192(N-1)S_3 - \frac{224}{3}(N-1)\zeta_3 - \frac{64P_{134}(N)S_2}{N(N+1)(N+2)^2(N-1)} \]
\[ - \frac{16P_{134}(N)}{N(N+1)(N+2)^2(N-1)} \zeta_2 \]
\[ + \frac{16P_{136}(N)}{3N^3(N+1)^3(N+2)^4(N-1)^3} \right\} , \quad \text{(D.168)} \]

with

\[ P_{134}(N) = 2N^6 + 6N^5 - 9N^4 + 16N^3 + 53N^2 + 8N - 4 , \quad \text{(D.169)} \]
\[ P_{135}(N) = N^{11} + 4N^{10} + 17N^9 + 58N^8 - 237N^7 - 278N^6 + 1057N^5 + 1156N^4 - 358N^3 - 420N^2 - 152N + 16 , \quad \text{(D.170)} \]
\[ P_{136}(N) = 4N^{15} + 22N^{14} + 79N^{13} + 95N^{12} - 575N^{11} + 335N^{10} + 3743N^9 - 3193N^8 - 13937N^7 - 1437N^6 + 10542N^5 + 3490N^4 - 832N^3 - 2752N^2 - 800N + 32 . \quad \text{(D.171)} \]

\[ \hat{A}_{Qg}^{(3),E2} = \frac{T_F^2 n_f C_A}{(N+1)^2(N+2)} \left\{ - \frac{1}{\varepsilon^3} \frac{32(2N^2 - 13N - 33)}{9(N-1)N} \right. \]
\[ + \left. \frac{1}{\varepsilon^2} \left[ - \frac{32}{9}S_1 + \frac{16P_{137}(N)}{27(N-1)^2N^2(N+1)(N+2)} \right] \right. \]
\[ + \left. \frac{1}{\varepsilon} \left[ - \frac{8(13N^2 - 79N - 198)}{9(N-1)N}S_2 - \frac{4(2N^2 - 13N - 33)}{3(N-1)N} \zeta_2 - \frac{8}{9}S_1^2 \right] \right. \]
\[ + \frac{16(26N^4 + 103N^3 + 253N^2 + 338N + 144)}{27(N-1)N(N+1)(N+2)}S_1 \]
\[
\begin{align*}
- \frac{8P_{138}(N)}{81(N-1)^3N^3(N+1)^2(N+2)^2} - \frac{8(5N^2 - 32N - 81)}{27(N-1)N} S_3 \\
+ \frac{28(2N^2 - 13N - 33)}{9(N-1)N} \zeta_3 - \frac{52}{9} S_2 S_1 - \frac{4}{3} \zeta_2 S_1 - \frac{4}{27} S_1^3 \\
+ \frac{4P_{139}(N)}{27(N-1)^2N^2(N+1)(N+2)} S_2 + \frac{2P_{140}(N)}{9(N-1)^2N^2(N+1)(N+2)} \zeta_2 \\
+ \frac{4(26N^4 + 103N^3 + 253N^2 + 338N + 144)}{27(N-1)N(N+1)(N+2)} S_1^2 \\
- \frac{8P_{141}(N)}{81(N-1)N(N+1)^2(N+2)^2} S_1 \\
+ \frac{4P_{142}(N)}{243(N-1)^4N^4(N+1)^3(N+2)^3} \bigg) , \quad (D.172)
\end{align*}
\]

with
\[
\begin{align*}
P_{137}(N) &= 52N^6 + 24N^5 + 28N^4 + 765N^3 + 532N^2 - 555N - 54 \ , \quad (D.173) \\
P_{138}(N) &= 572N^{10} + 1696N^9 + 2460N^8 + 207N^7 - 18024N^6 - 24537N^5 \\
&\quad + 16705N^4 + 20618N^3 - 12729N^2 - 900N - 324 \ , \quad (D.174) \\
P_{139}(N) &= 338N^6 + 221N^5 + 318N^4 + 4675N^3 + 2998N^2 - 3474N \\
&\quad - 324 \ , \quad (D.175) \\
P_{140}(N) &= 52N^6 + 24N^5 + 28N^4 + 765N^3 + 532N^2 - 555N - 54 \ , \quad (D.176) \\
P_{141}(N) &= 286N^6 + 1856N^5 + 5575N^4 + 8375N^3 + 4624N^2 - 1276N \\
&\quad - 1296 \ , \quad (D.177) \\
P_{142}(N) &= 4276N^{14} + 16804N^{13} + 10992N^{12} - 81178N^{11} - 181276N^{10} \\
&\quad + 209316N^9 + 783074N^8 - 83677N^7 - 1043730N^6 + 235534N^5 \\
&\quad + 660610N^4 - 261267N^3 - 4554N^2 - 6372N - 1944 \ . \quad (D.178)
\end{align*}
\]
\[
\begin{align*}
- \frac{2P_{145}(N)}{27(N - 1)N^2(N + 1)^3(N + 2)}S_2 &\quad - \frac{P_{146}(N)}{9(N - 1)N^2(N + 1)^3(N + 2)^2}\zeta_2 \\
- \frac{4P_{147}(N)}{81N^2(N + 1)^2(N + 2)^2}S_1 &\quad - \frac{2P_{148}(N)}{243(N - 1)^3N^4(N + 1)^5(N + 2)^3}\rightbrace, \\
\end{align*}
\]
with
\[
\begin{align*}
P_{143}(N) &= 46N^7 + 251N^6 + 255N^5 - 250N^4 + 234N^3 + 737N^2 \\
&\quad - 247N - 234, \quad (D.180) \\
P_{144}(N) &= 146N^{11} + 1928N^{10} + 4491N^9 + 869N^8 - 3135N^7 - 10143N^6 \\
&\quad - 26309N^5 - 3731N^4 + 25311N^3 + 4129N^2 - 4824N - 2988 \quad (D.181) \\
P_{145}(N) &= 281N^7 + 1541N^6 + 1589N^5 - 1441N^4 + 1400N^3 + 4328N^2 \\
&\quad - 1542N - 1404, \quad (D.182) \\
P_{146}(N) &= 46N^7 + 251N^6 + 255N^5 - 250N^4 + 234N^3 + 737N^2 - 247N \\
&\quad - 234, \quad (D.183) \\
P_{147}(N) &= 35N^6 - 243N^5 - 1303N^4 - 2082N^3 - 136N^2 + 2136N \quad + 720, \quad (D.184) \\
P_{148}(N) &= 454N^{15} + 15564N^{14} + 57172N^{13} + 34999N^{12} - 143229N^{11} \quad \\
&\quad - 317074N^{10} - 15876N^9 + 850116N^8 + 667430N^7 \quad - 871408N^6 - 712308N^5 + 468109N^4 + 287657N^3 \quad \\
&\quad + 51030N^2 - 79092N - 36936. \quad (D.185)
\end{align*}
\]
\[
z^{(3),G_2}_{Q_9} = \frac{T_{\Xi}n_fC_A}{N(N + 1)(N + 2)} \left\{ \frac{1}{\xi^3} \left[ \frac{32(N - 4)}{9}S_1 + \frac{32(N^2 + 2N + 4)}{9(N + 2)} \right] \right. \\
\left. + \frac{1}{\xi^2} \left[ \frac{8(N - 4)}{3}S_1^2 + \frac{8(N - 4)}{3}S_2 \\
- \frac{16(26N^4 - 16N^3 - 87N^2 - 83N - 128)}{27(N - 1)(N + 1)(N + 2)}S_1 \\
+ \frac{16P_{150}(N)}{27(N - 1)N(N + 1)(N + 2)^2} \right] \\
+ \frac{1}{\xi} \left[ \frac{28(N - 4)}{27}S_1^3 + \frac{4(N - 4)}{3}\zeta \xi S_1 + \frac{4(31N - 28)}{9}S_2S_1 \\
- \frac{16(7N + 12)}{9}S_2S_1 - \frac{8(17N + 28)}{27}S_3 \\
- \frac{4(28N^4 - 12N^3 - 35N^2 + 19N - 96)}{9(N - 1)(N + 1)(N + 2)}S_2^2 + \frac{4(N^2 + 2N + 4)}{3(N + 2)}\zeta_2 \right). 
\]
\[ \begin{align*}
&+ \frac{4(12N^4 + 172N^3 + 215N^2 - 159N - 144)}{9(N - 1)(N + 1)(N + 2)} S_2 \\
&+ \frac{8P_{151}(N)}{81(N - 1)(N + 1)^2(N + 2)^2} S_1 - \frac{8P_{152}(N)}{81(N - 1)N^2(N + 1)^2(N + 2)^2} S_2 \\
&+ \frac{5(N - 4)}{18} S_1^4 + (N - 4)ζ_2 S_1^2 + \frac{(29N - 20)}{3} S_2 S_1^2 - \frac{28(N - 4)}{9} ζ_3 S_1 \\
&+ \frac{20(5N - 4)}{9} S_3 S_1 - \frac{8(17N + 36)}{9} S_{2,1} S_1 + \frac{29(N - 4)}{6} S_2^2 \\
&- \frac{(181N + 204)}{9} S_4 - \frac{8(5N + 36)}{9} S_{3,1} \\
&- \frac{2(200N^4 - 76N^3 - 141N^2 + 337N - 608)}{81(N - 1)(N + 1)(N + 2)} S_3^3 \\
&- \frac{2(26N^4 - 16N^3 - 87N^2 - 83N - 128)}{9(N - 1)(N + 1)(N + 2)} ζ_2 S_1 + \frac{8(17N + 36)}{9} S_{2,1,1} \\
&- \frac{2(296N^4 - 940N^3 - 2133N^2 - 359N - 260)}{27(N - 1)(N + 1)(N + 2)} S_2 S_1 - \frac{28(N - 2 + 2N + 4)}{9(N + 2)} ζ_3 \\
&+ \frac{4(676N^4 + 2332N^3 + 1947N^2 - 2035N - 2632)}{81(N - 1)(N + 1)(N + 2)} S_3 \\
&+ \frac{8(2N^3 - 150N^2 - 491N - 384)}{27(N + 1)(N + 2)} S_{2,1} + (N - 4)ζ_2 S_2 \\
&+ \frac{2P_{149}(N)}{27(N - 1)(N + 1)^2(N + 2)^2} S_1^2 + \frac{2P_{150}(N)}{9(N - 1)N(N + 1)(N + 2)^2} ζ_2 \\
&- \frac{2P_{153}(N)}{27(N - 1)N(N + 1)^2(N + 2)^2} S_2 - \frac{4P_{154}(N)}{243(N - 1)(N + 1)^3(N + 2)^3} S_1 \\
&+ \frac{4P_{155}(N)}{243(N - 1)N^3(N + 1)^3(N + 2)^4} \right) ,
\end{align*} \]

with

\[ \begin{align*}
P_{149}(N) &= 242N^6 + 246N^5 - 495N^4 - 958N^3 - 2384N^2 - 1979N + 1296 ,
\end{align*} \]

\[ \begin{align*}
P_{150}(N) &= 13N^6 + 82N^5 + 16N^4 - 353N^3 - 446N^2 - 152N - 24 ,
\end{align*} \]

\[ \begin{align*}
P_{151}(N) &= 268N^6 + 412N^5 - 1147N^4 - 4532N^3 - 6520N^2 - 2513N + 1936 ,
\end{align*} \]

\[ \begin{align*}
P_{152}(N) &= 53N^9 + 341N^8 - 693N^7 - 6717N^6 - 13305N^5 - 8433N^4 + 2422N^3 + 4324N^2 + 1128N + 144 ,
\end{align*} \]

\[ \begin{align*}
P_{153}(N) &= 342N^7 + 3314N^6 + 8767N^5 + 8398N^4 + 2732N^3 + 879N^2 + 48N + 288 ,
\end{align*} \]

\[ \begin{align*}
P_{154}(N) &= 1940N^8 + 8156N^7 + 9782N^6 - 20076N^5 - 94500N^4 - 153048N^3 - 142667N^2 - 123635N - 76928 ,
\end{align*} \]

\[ \begin{align*}
P_{155}(N) &= 2833N^{12} + 32644N^{11} + 146294N^{10} + 316196N^9 + 266628N^8 - 211206N^7 - 715870N^6 - 709393N^5 - 362414N^4 - 119936N^3 - 36528N^2 - 8064N - 864 ,
\end{align*} \]
$$
\begin{align*}
\frac{z^{(3),H_2}}{A_{Qg}} &= \frac{T^{2}_f n_f C_A}{(N+1)^2(N+2)} \left\{ -\frac{1}{\varepsilon^3} \left[ \frac{32(2N^2 - 13N - 33)}{9(N-1)N} \right] \\
&+ \frac{1}{\varepsilon^2} \left[ -\frac{32}{9} S_1 + \frac{16 P_{156}(N)}{27(N-1)^2 N^2(N+1)(N+2)} \right] \\
&+ \frac{1}{\varepsilon} \left[ -\frac{8}{9} S_1^2 - \frac{8(13N^2 - 79N - 198)}{9(N-1)N} S_2 - \frac{4(2N^2 - 13N - 33)}{3(N-1)N} S_1 \right] \\
&+ \frac{16(26N^4 + 103N^3 + 253N^2 + 338N + 144)}{27(N-1)N(N+1)(N+2)} S_1 \right\} \\
&- \frac{8P_{157}(N)}{81(N-1)^3 N^3(N+1)^2(N+2)^2} - \frac{88(5N^2 - 32N - 81)}{27(N-1)N} S_3 \\
&+ \frac{28(2N^2 - 13N - 33)}{9(N-1)N} \zeta_3 - \frac{52}{9} S_2 S_1 - \frac{4}{3} \zeta_2 S_1 - \frac{4}{27} S_1^3 \\
&+ \frac{4(26N^4 + 103N^3 + 253N^2 + 338N + 144)}{27(N-1)N(N+1)(N+2)} S_1^2 \\
&+ \frac{27(N-1)^2 N^2(N+1)(N+2)}{2P_{159}(N)} S_2 \\
&+ \frac{8P_{160}(N)}{81(N-1)N(N+1)^2(N+2)^2} S_1 \\
&+ \frac{4P_{161}(N)}{243(N-1)^3 N^4(N+1)^3(N+2)^3} 
\right\} ,
\end{align*}
$$

with

$$
\begin{align*}
P_{156}(N) &= 52N^6 + 6N^5 - 26N^4 + 783N^3 + 658N^2 - 555N - 126 , \\
P_{157}(N) &= 572N^{10} + 1480N^9 + 1920N^8 + 1233N^7 - 15432N^6 \\
&- 26697N^5 + 12385N^4 + 23048N^3 - 10029N^2 - 1980N \\
&- 756 , \\
P_{158}(N) &= 338N^6 + 113N^5 - 6N^4 + 4783N^3 + 3754N^2 - 3474N \\
&- 756 , \\
P_{159}(N) &= 52N^6 + 6N^5 - 26N^4 + 783N^3 + 658N^2 - 555N - 126 , \\
P_{160}(N) &= 286N^6 + 1856N^5 + 5575N^4 + 8375N^3 + 4624N^2 - 1276N \\
&- 1296 , \\
P_{161}(N) &= 4276N^{14} + 15508N^{13} + 8400N^{12} - 72916N^{11} - 173500N^{10} \\
&+ 169140N^9 + 778700N^8 + 23729N^7 - 1060254N^6 \\
&+ 98482N^5 + 694468N^4 - 190635N^3 - 20106N^2 - 14148N \\
&- 4536 .
\end{align*}
$$
The individual contributions to $\hat{A}^\text{PS}_{Qq}$ are:

$$\hat{A}^{(3),\text{PS},a}_{Qq} = \frac{T_F^2 n_f C_F}{N^2(N+1)^2} \left\{ -\frac{1}{3} \left[ \frac{64}{9} (2+N)(-1+N) \right] \right.$$

$$+ \frac{1}{\varepsilon^2} \left[ -\frac{32}{9} (2+N)(-1+N)S_1 + \frac{32}{27} \frac{P_{162}(N)}{N(1+N)(2+N)} \right]$$

$$+ \frac{1}{\varepsilon} \left[ -\frac{104}{9} (2+N)(-1+N)S_2 I \frac{8}{9} (2+N)(-1+N)S_1 \right]$$

$$- \frac{8}{3} (2+N)(-1+N)\zeta_2 + \frac{16}{27} \frac{P_{162}(N)}{N(1+N)(2+N)} S_1$$

$$- \frac{16}{81} \frac{P_{163}(N)}{N^2(1+N)^2(2+N)^2} \right\}$$

$$- \frac{16}{81} \frac{P_{163}(N)}{N^2(1+N)^2(2+N)^2} - \frac{440}{27} (2+N)(-1+N)S_3$$

$$- \frac{52}{9} (2+N)(-1+N)S_2 S_1 - \frac{4}{27} (2+N)(-1+N)S_1^2$$

$$+ \frac{56}{9} (2+N)(-1+N)\zeta_3 - \frac{4}{3} (2+N)(-1+N)S_1 \zeta_2$$

$$+ \frac{52}{27} \frac{P_{162}(N)}{N(1+N)(2+N)} S_2 + \frac{4}{27} \frac{P_{162}(N)}{N(1+N)(2+N)} S_1^2$$

$$+ \frac{4}{9} \frac{P_{162}(N)}{N(1+N)(2+N)} \zeta_2 - \frac{8}{81} \frac{P_{163}(N)}{N^2(1+N)^2(2+N)^2} S_1$$

$$+ \frac{8}{243} \frac{P_{164}(N)}{N^3(1+N)^3(2+N)^3} \right\} , \quad (D.201)$$

with

$$P_{162}(N) = 8N^5 + 29N^4 - 9N^3 - 8N^2 + 64N + 24 , \quad (D.202)$$

$$P_{163}(N) = 25N^8 + 151N^7 + 116N^6 + 352N^5 + 1052N^4$$

$$- 428N^3 - 2264N^2 - 1200N - 288 , \quad (D.203)$$

$$P_{164}(N) = 158N^{11} + 1505N^{10} + 5261N^9 + 12912N^8 + 13860N^7$$

$$- 16140N^6 - 33344N^5 + 27880N^4 + 77344N^3$$

$$+ 50496N^2 + 19584N + 3456 . \quad (D.204)$$

$$\hat{A}^{(3),\text{PS},b}_{Qq} = \frac{T_F^2 n_f C_F}{(N-1)N(N+1)(N+2)} \left\{ \frac{1}{9} \frac{512}{\varepsilon^3} \right.$$

$$+ \frac{1}{\varepsilon^2} \left[ -\frac{256}{9} S_1 + \frac{1024}{27} \frac{2N^2 - 5}{(2+N)(1+N)} \right]$$
\[
+ \frac{1}{\varepsilon} \left[ -\frac{832}{9} S_2 - \frac{64}{9} S_1^2 - \frac{64}{3} \zeta_2 + \frac{512}{27} \frac{(2 N^2 - 5)}{(2 + N)(1 + N)} S_1 \right]
- \frac{128}{81} \frac{(25 N^4 - 42 N^3 - 107 N^2 + 348 N + 532)}{(2 + N)^2(1 + N)^2}
- \frac{3520}{27} S_3 - \frac{416}{9} S_2 S_1 - \frac{32}{27} S_1^3 - \frac{32}{3} S_1 \zeta_2 + \frac{448}{9} \zeta_3
+ \frac{1664}{27} \frac{(2 N^2 - 5)}{(2 + N)(1 + N)} S_2 + \frac{128}{27} \frac{(2 N^2 - 5)}{(2 + N)^2(1 + N)^2} S_1^2
+ \frac{128}{9} \frac{(2 N^2 - 5)}{(2 + N)(1 + N)} \zeta_2
- \frac{64}{81} \frac{(25 N^4 - 42 N^3 - 107 N^2 + 348 N + 532)}{(2 + N)^2(1 + N)^2} S_1
+ \frac{128}{243} \frac{P_{165}(N)}{(2 + N)^3(1 + N)^3} \right],
\]

with

\[
P_{165}(N) = 79 N^6 + 411 N^5 + 2085 N^4 + 5289 N^3 + 3252 N^2 - 5484 N - 6064.
\]

D.3 \( \hat{A}_{qq,Q}^{\text{PS}} \)

The contributions to \( \hat{A}_{qq,Q}^{\text{PS}} \) read:

\[
\hat{A}_{qq,Q}^{(3),\text{PS,a}} = \frac{T_F n_f C_F}{(N-1)N(N+1)(N+2)} \left\{ -\frac{1}{\varepsilon^3} \left[ \frac{512}{9} \right] + \frac{1}{\varepsilon^2} \left[ \frac{512}{9} S_1 - \frac{512(2N+1)(4N+7)}{27(N+1)(N+2)} \right] \right. \\
+ \frac{1}{\varepsilon} \left[ -\frac{256}{9} S_2 - \frac{64}{3} \zeta_2 + \frac{256}{9} S_1^2 + \frac{512(2N+1)(4N+7)}{27(N+1)(N+2)} S_1 \right] \\
- \frac{128}{81} \frac{(181 N^4 + 894 N^3 + 1597 N^2 + 1248 N + 400)}{(N+1)^2(N+2)^2} + \frac{256}{9} S_2 S_1 + \frac{64}{3} \zeta_2 S_1 \\
+ \frac{256}{27} S_1^3 + \frac{512}{27} S_3 + \frac{448}{9} \zeta_3 + \frac{(2N+1)(4N+7)}{(N+1)(N+2)} \left[ -\frac{256}{27} S_2^2 - \frac{256}{27} S_2 - \frac{64}{9} \zeta_2 \right] \\
+ \frac{128}{81} \frac{(181 N^4 + 894 N^3 + 1597 N^2 + 1248 N + 400)}{(N+1)^2(N+2)^2} S_1 \\
- \frac{128}{243} \frac{P_{166}(N)}{(N+1)^3(N+2)^3} \right\},
\]

with

\[
P_{166}(N) = 1037 N^6 + 8247 N^5 + 26940 N^4 + 46191 N^3 + 43809 N^2 \\
+ 21648 N + 4192.
\]
\[ \hat{A}_{qq,Q}^{(3),PS,b} = \frac{T_F^2 n_f C_F}{N^2 (N+1)^2} \left\{ \frac{1}{\varepsilon^3} \begin{array}{c} -\frac{64}{9} (2+N)(-1+N) \\ + \frac{1}{\varepsilon^2} \begin{array}{c} \frac{64}{9} (2+N)(-1+N) S_1 \\ - \frac{32}{27} \frac{16 N^4 + 26 N^3 - 25 N^2 - 11 N + 6}{N(1+N)} \\ + \frac{1}{\varepsilon} \begin{array}{c} - \frac{32}{9} S_2 - \frac{32}{9} S_1^2 - \frac{8}{3} \zeta_2 \\ + \frac{32}{27} \frac{16 N^4 + 26 N^3 - 25 N^2 - 11 N + 6}{N(1+N)} S_1 - \frac{16}{81} \frac{P_{167}(N)}{N^2(1+N)^2} \end{array} \\ + (N+2)(N-1) \left( \frac{64}{27} S_3 + \frac{32}{9} S_2 S_1 + \frac{32}{27} S_1^3 + \frac{8}{3} S_1 \zeta_2 + \frac{56}{9} \zeta_3 \right) - \frac{16}{27} \frac{(16 N^4 + 26 N^3 - 25 N^2 - 11 N + 6)}{N(1+N)} S_2 - \frac{16}{27} \frac{(16 N^4 + 26 N^3 - 25 N^2 - 11 N + 6)}{N(1+N)} S_1^2 - \frac{4}{9} \frac{(16 N^4 + 26 N^3 - 25 N^2 - 11 N + 6)}{N(1+N)} \zeta_2 + \frac{16}{81} \frac{P_{167}(N)}{N^2(1+N)^2} S_1 - \frac{8}{243} \frac{P_{168}(N)}{N^3(1+N)^3} \end{array} \right\}, \] (D.209)

with

\[ P_{167}(N) = 181 N^6 + 447 N^5 - 32 N^4 - 297 N^3 - 92 N^2 + 15 N - 18, \quad \] (D.210)
\[ P_{168}(N) = 2074 N^8 + 7210 N^7 + 4927 N^6 - 3503 N^5 - 5309 N^4 - 929 N^3 + 231 N^2 + 9 N + 54. \] (D.211)

D.4 \( \hat{A}_{qq,Q}^{NS} \)

The contributions to \( \hat{A}_{qq,Q}^{NS} \) are given by :

\[ \hat{A}_{qq,Q}^{(3),NS,a} = \frac{T_F^2 n_f C_F}{N(N+1)} \left\{ -\frac{1}{\varepsilon^3} \begin{array}{c} \frac{64}{27} (N+2)(N-1) \\ - \frac{1}{\varepsilon^2} \begin{array}{c} \frac{64}{81} (N^4 + 2 N^3 - 10 N^2 - 5 N + 3) \\ + \frac{1}{\varepsilon} \begin{array}{c} - \frac{8}{9} (N+2)(N-1) \zeta_2 - \frac{8}{3} \frac{P_{169}(N)}{1 + N^2} \\ - \frac{8}{243} \frac{P_{168}(N)}{N^3(1+N)^3} \end{array} \end{array} \end{array} \right\}, \]
\[
\begin{align*}
\frac{56}{27} (N + 2)(-1 + N) \zeta_3 & - \frac{8}{27} \left( -5 N - 10 N^2 + 2 N^3 + N^4 + 3 \right) \frac{1}{(1 + N)^{1/4}} \zeta_2 \\
- \frac{16}{729} \frac{P_{170}(N)}{(1 + N)^2 N^3} \right\}, \\
\end{align*}
\]

with

\[
\begin{align*}
P_{169}(N) & = +14 N^6 + 42 N^5 - N^4 - 50 N^3 - 19 N^2 + 2 N - 3, \quad (D.213) \\
P_{170}(N) & = +308 N^8 + 1232 N^7 + 395 N^6 - 2353 N^5 - 2413 N^4 \\
& - 391 N^3 + 153 N^2 + 9 N + 27. \\ 
\end{align*}
\]

\[
\hat{A}_{qq,Q}^{(3),NS,b} = T_F^2 n_f C_F \left\{ \begin{array}{c}
\frac{1}{\varepsilon^3} \left[ -\frac{128}{27} S_1 + \frac{128}{27} \right] + \frac{1}{\varepsilon^2} \left[ \frac{128}{81} + \frac{64}{27} S_2 - \frac{320}{81} S_1 \right] \\
+ \frac{1}{\varepsilon} \left[ -\frac{32}{27} S_3 - \frac{16}{9} \zeta_2 S_1 + \frac{160}{81} S_2 + \frac{16}{9} \zeta_2 - \frac{320}{27} S_1 + \frac{896}{81} \right] \\
+ \frac{16}{27} S_4 + \frac{112}{27} \zeta_3 S_1 + \frac{8}{9} \zeta_2 S_3 - \frac{80}{81} S_3 + \frac{112}{27} \zeta_3 - \frac{40}{27} \zeta_2 S_1 \\
+ \frac{16}{27} \zeta_2 + \frac{160}{27} S_2 - \frac{13888}{729} S_1 + \frac{9856}{729} \end{array} \right\}. \\
\end{align*}
\]

\[
\hat{A}_{qq,Q}^{(3),NS,c} = T_F^2 n_f C_F \left\{ -\frac{1}{\varepsilon^2} \frac{16}{9} - \frac{1}{\varepsilon} \frac{120}{27} - \frac{2}{3} \zeta_2 - \frac{337}{81} \right\}. \\
\]

**D.5** \(A_{qq,Q}^{NS,TR}\)

The contributions to \(\hat{A}_{qq,Q}^{NS,TR}\) read:

\[
\hat{A}_{qq,Q}^{(3),TR,a} = T_F^2 n_f C_F \left\{ -\frac{1}{\varepsilon^3} \frac{164}{27} - \frac{1}{\varepsilon^2} \frac{164}{81} - \frac{1}{\varepsilon} \left[ \frac{32(14 N^2 + 14 N - 3)}{81 N(N + 1)} + \frac{8}{9} \zeta_2 \right] \\
- \frac{16}{729} \frac{P_{170}(N)}{(1 + N)^2 N^3 (N + 1)^2} \right\}.
\]

\[
\hat{A}_{qq,Q}^{(3),TR,a} = T_F^2 n_f C_F \left\{ -\frac{1}{\varepsilon^3} \frac{164}{27} - \frac{1}{\varepsilon^2} \frac{164}{81} - \frac{1}{\varepsilon} \left[ \frac{32(14 N^2 + 14 N - 3)}{81 N(N + 1)} + \frac{8}{9} \zeta_2 \right] \\
+ \frac{56}{27} \zeta_3 \right\}. \\
\]

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\[ A^{(3),TR,b}_{q,q,Q} = T_F^2 n_f C_F \left\{ \frac{1}{\epsilon^3} \left[ -\frac{128}{27} S_1 + \frac{128}{27} \right] + \frac{1}{\epsilon^2} \left[ \frac{64}{27} S_2 - \frac{320}{81} S_1 + \frac{128}{81} \right] \right. \\
+ \frac{1}{\epsilon} \left[ -\frac{32}{27} S_3 - \frac{16}{9} \zeta_2 S_1 + \frac{160}{81} S_2 + \frac{16}{9} \zeta_2 - \frac{320}{27} S_1 + \frac{896}{81} \right] \right. \\
+ \frac{16}{27} S_4 + \frac{112}{27} \zeta_3 S_1 + \frac{8}{9} \zeta_2 S_2 - \frac{80}{81} S_3 - \frac{40}{27} \zeta_2 S_1 - \frac{112}{27} \zeta_3 + \frac{160}{27} S_2 \\
+ \frac{16}{27} \zeta_2 - \frac{13888}{729} S_1 + \frac{9856}{729} \right\}. \quad (D.218) \]

\[ A^{(3),TR,c}_{q,q,Q} = T_F^2 n_f C_F \left\{ \frac{1}{\epsilon^2} \frac{16}{9} - \frac{1}{\epsilon} \frac{20}{27} - \frac{2}{3} \zeta_2 - \frac{337}{81} \right\}. \quad (D.219) \]
E Variable Transformations

In many cases the structure of the emerging Feynman parameter integrals can be simplified by applying transformations to the integration variables, which were given in Ref. [217].

• To define the product \( x' = xy \) as the new integration variable, one maps:

\[
x' \; := \; xy \quad \text{and} \quad y' \; := \; \frac{x(1-y)}{1-xy},
\]
\[
x = x' + y' - x'y' \quad \text{and} \quad y = \frac{x'}{y' + x' - x'y'},
\]
\[
\frac{\partial(x,y)}{\partial(x',y')} = \frac{1-x'}{x' + y' - x'y'}. \tag{E.1}
\]

One obtains

\[
\int_0^1 \int_0^1 dx\,dy \; f(x,y)(xy)^N = \int_0^1 \int_0^1 dx'\,dy' \; \frac{(1-x')(x')^N}{x' + y' - x'y'} \cdot f \left( y' + x' - x'y', \frac{x'}{x' + y' - x'y'} \right). \tag{E.2}
\]

• Terms of the form \((x - y)^N\) can be combined by

\[
x > y : \quad x' := x - y, \quad y' := \frac{y}{1-x+y},
\]
\[
x < y : \quad x' := y - x, \quad y' := \frac{1-y}{1+x-y},
\]
\[
x = x' + y' - x'y', \quad y = (1-x')y', \quad \frac{\partial(x,y)}{\partial(x',y')} = 1 - x'. \tag{E.3}
\]

Thus, one obtains

\[
\int_0^1 \int_0^1 dx\,dy \; f(x,y)(x-y)^N = \int_0^1 \int_0^1 dx'\,dy' \cdot x'^N \left[ f(y' + x' - x'y', (1-x')y') + (-1)^N f((1-x')y')(1-x'), 1 - (1-x')y' \right]. \tag{E.4}
\]

If one applies Eq. (E.3) to factors \((x - y)\) in the denominator, special care is needed to avoid possible divergences. The above transformations allow to simplify the Feynman parameter integrals analytically. In this way higher transcendental functions like generalized hypergeometric functions, which obey single-sum representations are obtained, cf. Eq. (F.11).
F Special Functions

In the following we summarize for convenience some relations for special functions which occur repeatedly in quantum field theory calculations and are mutually used within the present work.

F.1 The Euler Integrals

The Γ-function, cf. [218, 219], is analytic in the whole complex plane except at the non-negative integers, where it possesses single poles. Euler’s infinite product defines

\[ \frac{1}{\Gamma(z)} = z \exp(\gamma_E z) \prod_{i=1}^{\infty} \left( 1 + \frac{z}{i} \right) \exp \left( -\frac{z}{i} \right) . \] (F.1)

The residues of the Γ-function at its poles are given by

\[ \text{Res}[\Gamma(z)]_{z=-N} = \frac{(-1)^N}{N!} , \quad N \in \mathbb{N} \cup 0 . \] (F.2)

In case of \( \text{Re}(z) > 0 \), the Γ-function can be expressed by Euler’s integral

\[ \Gamma(z) = \int_0^{\infty} dt \exp(-t) t^{z-1} , \] (F.3)

from which one infers the well known functional equation of the Γ-function

\[ \Gamma(z+1) = z\Gamma(z) , \] (F.4)

which may be used for its analytic continuation. Around \( z = 1 \), the following series expansion is obtained

\[ \Gamma(1-\varepsilon) = \exp(\varepsilon \gamma_E) \exp \left\{ \sum_{i=2}^{\infty} \zeta_i \frac{\varepsilon^i}{i} \right\} , \quad |\varepsilon| < 1 . \] (F.5)

Here and in (F.1), \( \gamma_E \) denotes the Euler-Mascheroni constant, cf. (C.8), and \( \zeta_k \) Riemann’s \( \zeta \)-function for integer arguments \( k \), cf. (C.10). A shorthand notation for rational functions of Γ–functions is

\[ \Gamma \left[ \begin{array}{c} a_1, \ldots, a_i \\ b_1, \ldots, b_j \end{array} \right] := \frac{\Gamma(a_1) \ldots \Gamma(a_i)}{\Gamma(b_1) \ldots \Gamma(b_j)} . \] (F.6)

Functions closely related to the Γ-function are the Euler Beta-function \( B(A, C) \) function, the \( \psi(x) \)--, and the \( \beta(x) \)--function.

The Beta-function can be defined by Eq. (F.6)

\[ B(A, C) = \Gamma \left[ \begin{array}{c} A, C \\ A + C \end{array} \right] . \] (F.7)

If \( \text{Re}(A), \text{Re}(C) > 0 \), the following integral representation is valid

\[ B(A, C) = \int_0^1 dx \; x^{A-1}(1 - x)^{C-1} . \] (F.8)
For arbitrary values of $A$ and $C$, (F.8) can be continued analytically outside of the respective singularities using Eqs. (F.1, F.7). Its expansion around singularities can be performed via Eqs. (F.2, F.5). The $\psi$-function and $\beta(x)$ are defined as logarithmic derivatives of the $\Gamma$-function via

$$
\psi(x) = \frac{1}{\Gamma(x)} \frac{d}{dx} \Gamma(x) , \\
\beta(x) = \frac{1}{2} \left[ \psi\left(\frac{x + 1}{2}\right) - \psi\left(\frac{x}{2}\right) \right].
$$

**(F.9)**

**(F.10)**

### F.2 The Generalized Hypergeometric Functions

The generalized hypergeometric function $pF_q$ is defined by, cf. [136, 137, 220],

$$
pF_q\left[ a_1, \ldots, a_P; b_1, \ldots, b_Q; z \right] = \sum_{i=0}^{\infty} \frac{(a_1)_i \cdots (a_P)_i}{(b_1)_i \cdots (b_Q)_i} \frac{z^i}{\Gamma(i+1)} .
$$

**(F.11)**

Here $(c)_n$ denotes Pochhammer’s symbol

$$
(c)_n = \frac{\Gamma(c + n)}{\Gamma(c)} ,
$$

**(F.12)**

for which the following relation holds

$$
(N + 1)_-^i = \frac{(-1)^i}{(-N)_i} , \quad N \in \mathbb{N} .
$$

**(F.13)**

In (F.11), there are $P$ numerator parameters $a_1 \ldots a_P$, $Q$ denominator parameters $b_1 \ldots b_Q$, and one variable $z$, all of which may be real or complex. Additionally, the denominator parameters must not be negative integers, since in that case (F.11) is not defined. The generalized hypergeometric series $pF_q$ are evaluated at a certain value of $z$, which is always $z = 1$ for the final expressions in this thesis.

Gauß was the first to study this kind of functions, introducing the function $2F_1$, and proving the theorem, cf. [136],

$$
2F_1[a, b; c; 1] = \Gamma\left[ \begin{array}{c} c, c - a - b \\ c - a, c - b \end{array} \right] , \quad \text{Re}(c - a - b) > 0 ,
$$

**(F.14)**

which is called Gauß’ theorem. An integral representation for the hypergeometric Gauß-function is given by

$$
2F_1\left[ \begin{array}{c} a, b + 1 \\ c + b + 2 \end{array}; z \right] = \Gamma\left[ \begin{array}{c} c + b + 2 \\ c + 1, b + 1 \end{array} \right] \int_0^1 dx \ x^b (1 - x)^c (1 - zx)^{-a} ,
$$

**(F.15)**

cf. [136], provided that the conditions

$$
|z| < 1 , \quad \text{Re}(c + 1), \text{Re}(b + 1) > 0 ,
$$

**(F.16)**

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hold. Applying Eq. (F.15) recursively, one obtains the following integral representation for the general hypergeometric function \(_{p+1}F_p\):

\[
_{p+1}F_p \left[ \begin{array}{c} a_0, a_1, \ldots, a_p \\ b_1, \ldots, b_p \end{array} ; z \right] = \Gamma \left[ \begin{array}{c} b_1, \ldots, b_p \\ a_1, \ldots, a_p, b_1 - a_1, \ldots, b_p - a_p \end{array} \right] \times \\
\int_0^1 dx_1 \cdots \int_0^1 dx_p \ x_1^{a_1-1}(1-x_1)^{b_1-a_1-1} \cdots x_p^{a_p-1}(1-x_p)^{b_p-a_p-1}(1-zx_1 \cdots x_p)^{-a_0} \, ,
\]

under similar conditions as in Eq. (F.16). As generalized hypergeometric functions appeared frequently during this computation, taking advantage of their properties is of importance.

If one considers the fraction

\[
\frac{(m)_i}{(n)_i} ,
\]

with integers \(m > n > 1\) one may transform the arguments in the following way by using the definition of Pochhammer’s symbol :

\[
\frac{(m)_i}{(n)_i} = \frac{\Gamma(n)}{\Gamma(m)} \frac{\Gamma(m+i-1)}{\Gamma(n+i-1)} \frac{m+i-1}{n+i-1} \\
= \frac{\Gamma(n) \Gamma(m+i-1)}{\Gamma(m) \Gamma(n+i-1)} \left(1 + \frac{m-n}{n-1+i} \right) \\
= \frac{\Gamma(n) \Gamma(m-1)}{\Gamma(m)} \frac{(m-1)_i}{(n-1)_i} \left[ \frac{1}{(n-1)_i \Gamma(n-1)} + \frac{(m-n) \Gamma(N)}{(n)_i} \right] \\
= \frac{m-1}{n-1} \frac{(m-1)_i}{(n-1)_i} + \frac{m-n}{m-1} \frac{(m-1)_i}{(n)_i} \tag{F.19}
\]

This relation can be applied to an arbitrary function \(pF_q\) and proves to be especially useful if one considers the generalized hypergeometric function \(_3F_2\) of the form \(_3F_2 \left[ \begin{array}{c} a_1, a_2, m \\ b_1, n \end{array} ; 1 \right] \), with \(m, n\) integers, \(n > m > 0\). In this case repeated application of

\[
_{3}F_{2} \left[ \begin{array}{c} a_1, a_2, m \\ b_1, n \end{array} ; z \right] = \frac{n-1}{m-1} \ _{3}F_{2} \left[ \begin{array}{c} a_1, a_2, m-1 \\ b_1, n-1 \end{array} ; 1 \right] \\
+ \frac{m-n}{m-1} \ _{3}F_{2} \left[ \begin{array}{c} a_1, a_2, m-1 \\ b_1, n \end{array} ; 1 \right] \tag{F.20}
\]

leads to a linear combination of terms of the form

\[
_{3}F_{2} \left[ \begin{array}{c} a_1, a_2, 1 \\ b_1, n \end{array} ; 1 \right] \tag{F.21}
\]

and terms that do not contain any sum any longer. These relations belong to the class of contiguous relations [136, 220–223]. If \(a_1, a_2, b_1\) are non–integers or \(a_1, a_2, b_1 > n - 1\)
(F.21) can be simplified by considering the following relations:

\[
\frac{1}{(n)_i} = \frac{\Gamma(n)}{\Gamma(n+i)} \frac{\Gamma(n)}{(n+i-1)!},
\]

\[
(A) = \frac{\Gamma(A+i)}{\Gamma(A)} = \frac{\Gamma(A+i-(n-1)+(n-1))}{\Gamma(A)}
\]

\[
= \frac{\Gamma(A-(n-1))}{\Gamma(A)} (A+1-n)_{i+n-1}.
\]

After applying (F.22) and (F.23) one obtains

\[
_3F_2 \left[ \begin{array}{c} a_1, a_2, 1 \\ b_1, n \end{array} ; 1 \right] = \sum_{i=0}^{\infty} \frac{(a_1)_i(a_2)_i}{(b_1)_i} \left( \frac{1}{(n)_i} \right)
\]

\[
= \frac{\Gamma(a_1+1-n)\Gamma(a_2+1-n)\Gamma(b_1)}{\Gamma(a_1)\Gamma(a_2)\Gamma(b_1+1-n)}
\]

\[
\sum_{i=0}^{\infty} \frac{(a_1+1-n)_i(a_2+1-n)_i}{(b_1+1-n)_i} \frac{1}{(n+i-1)!}
\]

\[
= \frac{\Gamma(a_1+1-n)\Gamma(a_2+1-n)\Gamma(b_1)}{\Gamma(a_1)\Gamma(a_2)\Gamma(b_1+1-n)}
\]

\[
\times \left\{ \frac{2F_1 \left[ \begin{array}{c} a_1+1-n, a_2+1-n \\ b_1+1-n \end{array} ; 1 \right] - \sum_{i=0}^{n-2} \frac{(a_1+1-n)_i(a_2+1-n)_i}{(b_1+1-n)_i} \frac{1}{(i)!} }{\Gamma(b_1+1-n)} \right\}.
\]

The infinite sum contained inside the hypergeometric function in (F.24) can now be evaluated by applying Gauß’ theorem, (F.14), such that no infinite sum remains. The relations (F.20) and (F.24) have been implemented into FORM-algorithms and in many cases made it possible to perform the infinite sums before expanding in the dimensional regularization parameter \( \varepsilon \). A similar useful relation is the following, which has been given in Ref. [224] and holds under the condition, that \( \text{Re}(e-a-b-1-k) > 0 \):

\[
_3F_2 \left[ \begin{array}{c} a, b, d+k \\ d, e \end{array} ; 1 \right] = \Gamma \left[ \begin{array}{c} e \\ e-a, e-b \end{array} \right] \sum_{i=0}^{k} \frac{\Gamma(e-a-b-i)}{\Gamma(i)} \frac{(a)_i(b)_i}{(d)_i}.
\]

The following relations are restricted to special cases, but prove often to be useful. One defines the parametric excess of the series by \( s := d+e-a-b-c \). Saalschütz’s theorem, cf. [136], states that

\[
_3F_2 \left[ \begin{array}{c} a, b, c \\ d, e \end{array} ; 1 \right] = \Gamma \left[ \begin{array}{c} d, 1+a-e, 1+b-e, 1+c-e \\ 1-e, d-a, d-b, d-c \end{array} \right],
\]

provided that \( s = 1 \), i.e. the series is Saalschützian, and one of the numerator parameters is equal to a negative integer. Another theorem is a generalization of Dixon’s theorem,
F.3 Harmonic Sums and Nielsen–Integrals

Expanding the \( \Gamma \)-function in \( \varepsilon \), its logarithmic derivatives, the \( \psi^{(k)} \)-functions, emerge. In many applications of perturbative QCD and QED, harmonic sums occur, cf. [124, 125], which can be considered as generalization of the \( \psi \)-function and the \( \beta \)-function. These are defined by

\[
S_{a_1, \ldots ,a_m}(N) = \sum_{n_1=1}^{N} \cdots \sum_{n_m=1}^{N} \frac{(\text{sign}(a_1))^{n_1}}{n_1^{a_1}} \frac{(\text{sign}(a_2))^{n_2}}{n_2^{a_2}} \cdots \frac{(\text{sign}(a_m))^{n_m}}{n_m^{a_m}},
\]

\( N \in \mathbb{N}, \forall l a_l \in \mathbb{Z} \setminus 0 \),

\( S_0 = 1 \).

We adopt the convention

\[
S_{a_1, \ldots ,a_m} \equiv S_{a_1, \ldots ,a_m}(N),
\]

i.e. harmonic sums are taken at argument \( N \), if no argument is indicated. Related quantities are the \( Z \)-sums defined by

\[
Z_{m_1, \ldots ,m_k}(N) = \sum_{N\geq i_1>i_2>\cdots>i_k>0} \prod_{l=1}^{k} \frac{[\text{sign}(m_i)]^{i_l}}{i_l^{[m_i]}}.
\]

The depth \( d \) and the weight \( w \) of a harmonic sum are defined by

\[
d := m,
\]

\[
w := \sum_{i=1}^{m} |a_i|.
\]

Harmonic sums of depth \( d = 1 \) are referred to as single harmonic sums. The complete set of algebraic relations connecting harmonic sums to other harmonic sums of the same or lower weight is known [131]. Thus the number of independent harmonic sums can be reduced significantly, e.g., up to \( w = 4 \) the 80 possible harmonic sums can be expressed algebraically in terms of 31 basic harmonic sums only [132]. One introduces a product for the harmonic sums, the shuffle product \( \sqcup \sqcup \), cf. [131]. For the product of a single and a general finite harmonic sum it is given by

\[
S_{a_1}(N) \sqcup \sqcup S_{b_1, \ldots ,b_m}(N) = S_{a_1,b_1, \ldots ,b_m}(N) + S_{b_1,a_1,b_2, \ldots ,b_m}(N) + \cdots + S_{b_1,b_2, \ldots ,b_m,a_1}(N).
\]

For sums \( S_{a_1, \ldots ,a_n}(N) \) and \( S_{b_1, \ldots ,b_m}(N) \) of arbitrary depth, the shuffle product is then the sum of all harmonic sums of depth \( m+n \) in the index set of which \( a_i \) occurs left of \( a_j \) for

[136],

\[
3F_2 \left[ \begin{array}{c} a, b, c \\ d, e; 1 \end{array} \right] = \Gamma \left[ \begin{array}{c} d, e, s \\ a, b + s, c + s; 1 \end{array} \right] 3F_2 \left[ \begin{array}{c} d - a, e - a, s \\ s + b, s + c; 1 \end{array} \right].
\]
\[ i < j, \text{ likewise for } b_k \text{ and } b_l \text{ for } k < l. \] Note that the shuffle product is symmetric. One shows that the following relation holds, cf. [131],

\[
S_{a_1}(N) \cdot S_{b_1, \ldots, b_m}(N) = S_{a_1}(N) \shuffle S_{b_1, \ldots, b_m}(N) \\
- S_{a_1 \land b_1, b_2, \ldots, b_m}(N) - \ldots - S_{b_1, b_2, \ldots, a_1 \land b_m}(N), \quad (F.35)
\]

where the \( \land \) symbol is defined as

\[
a \land b = \text{sign}(a) \text{sign}(b) \ (|a| + |b|). \quad (F.36)
\]

Due to the additional terms containing wedges (\( \land \)) between indices, harmonic sums form a quasi–shuffle algebra, [225,226]. By summing (F.35) over permutations, one obtains the symmetric algebraic relations between harmonic sums. At depth 2 and 3 these read, [124],

\[
S_{m,n} + S_{n,m} = S_m S_n + S_{m \land n}, \quad (F.37)
\]

\[
\sum_{\text{perm\{l,m,n\}}} S_{l,m,n} = S_l S_m S_n + \sum_{\text{inv\ perm\{l,m,n\}}} S_l S_{m \land n} + 2 S_{l \land m \land n}, \quad (F.38)
\]

which we used extensively to simplify our expressions. In (F.37, F.38), “perm” denotes all permutations and “inv\ perm” invariant ones.

The limit \( N \to \infty \) of finite harmonic sums exists only if \( a_1 \neq 1 \) in (F.28). Additionally, one defines all \( \sigma \)-values symbolically as

\[
\sigma_{k_1, \ldots, k_l} = \lim_{N \to \infty} S_{a_1, \ldots, a_l}(N). \quad (F.39)
\]

The finite \( \sigma \)-values are related to multiple \( \zeta \)-values, [124,125,134,135,202,227,228]. Further we define the symbols

\[
\sigma_0 := \sum_{i=1}^{\infty} \frac{1}{i}, \quad (F.40)
\]

\[
\sigma_1 := \sum_{i=1}^{\infty} 1. \quad (F.41)
\]

It is useful to include these \( \sigma \)-values into the algebra, since they allow to treat parts of sums individually, accounting for the respective divergences, cf. also [124,125,202]. These divergent pieces cancel in the end if the overall sum is finite.

The relation of single harmonic sums with positive or negative indices to the \( \psi^{(k)} \)–functions is then given by

\[
S_1(N) = \psi(N+1) + \gamma_E, \quad (F.42)
\]

\[
S_a(N) = \frac{(-1)^{a-1} \psi^{(a-1)}(N+1) + \zeta_a}{\Gamma(a)}, \quad k \geq 2, \quad (F.43)
\]

\[
S_{-1}(N) = (-1)^N \beta(N+1) - \ln(2), \quad (F.44)
\]

\[
S_{-a}(N) = -\frac{(-1)^{N+a}}{\Gamma(a)} \beta^{(a-1)}(N+1) - (1 - 2^{1-a}) \zeta_a, \quad k \geq 2. \quad (F.45)
\]

Single harmonic sums can be analytically continued to complex values of \( N \) by these relations. At higher depths, harmonic sums can be expressed in terms of Mellin–transforms of

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polylogarithms and the more general Nielsen-integrals, [229–231]. The latter are defined by

\[ S_{n,p}(z) = \frac{(-1)^{n+p-1}}{(n-1)! p!} \int_0^1 \frac{dx}{x} \log^{n-1}(x) \log^p(1 - zx) \]  
\[ \text{(F.46)} \]

and fulfill the relation

\[ \frac{dS_{n,p}(x)}{d \log(x)} = S_{n-1,p}(x) . \]  
\[ \text{(F.47)} \]

If \( p = 1 \), one obtains the polylogarithms

\[ \text{Li}_n(x) = S_{n-1,1}(x) , \]  
\[ \text{(F.48)} \]

where

\[ \text{Li}_0(x) = \frac{x}{1 - x} . \]  
\[ \text{(F.49)} \]

These functions do not suffice for arbitrary harmonic sums, in which case the harmonic polylogarithms have to be considered, [232]. The latter functions obey a direct shuffle algebra, cf. [131–134, 202]. The representation in terms of Mellin–transforms then allows an analytic continuation of arbitrary harmonic sums to complex \( N \), cf. [233–236]. Equivalently, one may express harmonic sums by factorial series, [219, 237, 238], up to polynomials of \( S_1(N) \) and harmonic sums of lower degree, and use this representation for the analytic continuation to \( N \in \mathbb{C} \), cf. [132, 133, 202].
G  Examples for Sums

In the present calculation numerous single- to triple finite and infinite sums of an extension of the hypergeometric type had to be calculated. For these sums, depending on various summation parameters, \( n_i \), the ratio of the summands, except the part containing harmonic sums,

\[
a(..., n_i + 1, ...) \quad \text{or} \quad \frac{a(..., n_i, ...)}{a(..., n_i + 1, ...)} , \quad \forall i
\]

is a rational function in all variables \( n_i \). Sums of this type can be represented by basic sums of a certain type, which are transcendental to each other and form sum- and product- fields, cf. [140–143] and references therein. The general form of these sums is

\[
\sum_{k_1=1}^{N_1(N)} \sum_{k_2=1}^{N_2(k_1,N)} \sum_{k_3=1}^{N_3(k_2,k_1,N)} R(k_1, k_2, k_3, N) \prod_{l=1}^{4} S_{a_l}(s(k_i, N)) \Gamma \left[ s_1(k_i, N) \ldots s_p(k_i, N) \right] \quad \text{(G.2)}
\]

with \( R \) a rational function, \( s(k_i, N) \) a linear combination of the arguments with weight \( \pm 1 \), \( a_l \) an index set, \( p, q \in \mathbb{N} \), \( N_i \in \mathbb{N} \cup \mathbb{\infty} \). The generalized \( \Gamma \)-function usually includes both Beta–functions and binomials.

In the present calculation one faces more complicated sums than occurring in earlier two–loop calculations up to \( O(\varepsilon) \), [120,121]. We present a few examples.

\[
\sum_{j_1=1}^{N-2} \sum_{n=1}^{\infty} (-1)^{j_1} B(n, N - j_1) \binom{N-2}{j_1} \frac{S_2(-j_1 + n + N)}{n^2(j_1 - N - 2)} =
\]

\[
\left\{ (-1)^N \frac{6 - 23N + 9N^2 + 2N^3}{2(N-1)^2N^2(1+N)(2+N)} + \left[ \frac{1}{N + 2} - \frac{27(-1)^N}{(N-1)(N+1)(N+2)} \right] S_1 \right. 
\]

\[
- \frac{1}{N(N+2)} \left. \right\} S_2^2
\]

\[
\left. + \frac{1}{N + 2} - \frac{48(-1)^N}{(N-1)(N+1)(N+2)} \right] S_3S_2 - \frac{2S_{2-2}}{N(N+2)}
\]

\[
\left. + \left\{ (-1)^N \frac{7(12 + 6N - 37N^2 + 6N^3 + N^4)}{20(-1 + N)^2N^2(1+N)(2+N)} + \frac{21}{5(-1 + N)(N+1)(2+N)} \right. \right]
\]

\[
- \frac{7}{10(N+2)} S_1 + \frac{7}{10N(N+2)} \right\} \zeta_2^2 + \left\{ (-1)^N \frac{6 - 23N + 9N^2 + 2N^3}{2(-1 + N)^2N^2(1+N)(2+N)} \right.
\]

\[
+ \frac{3(-1)^N}{(N-1)N(N+1)(N+2)} + \frac{3}{N + 2} \left. \right\} \left. \right] S_4 - \frac{3}{N(N+2)} \right]
\]

\[
+ \frac{3}{N + 2} - \frac{18(-1)^N}{(N-1)N(N+1)(N+2)} \right) \right]
\]

\[
S_5 + \left[ \frac{2S_{2-2}}{N + 2} + \frac{(-1)^N(3N-1)}{(N-1)^3N^3} \right] S_1
\]

\[
+ \frac{2}{2 + N} S_{2}S_{3} + \left\{ (-1)^N \frac{3(12 - 6N - 14N^2 + 7N^3 + 12N^4 + N^5)}{(-1 + N)^3N^3(1+N)(2+N)} \right.
\]
\[
\begin{align*}
&\frac{9 S_1^2}{(1 + N) N (1 + N) (2 + N)} + (-1)^N \frac{3 (6 - 23 N + 9 N^2 + 2 N^3)}{(1 + N)^2 N^2 (1 + N) (2 + N) S_1} \biggr) \\
&+ \left[ \frac{3 (-1)^N}{(N - 1) N (N + 1) (N + 2)} - \frac{1}{N + 2} \right] S_{2,1} \\
&+ \left[ (-1)^N \frac{2 (12 - 37 N + 9 N^2 + 4 N^3)}{(1 + N) N^2 (1 + N) (2 + N)} + (-1)^N \frac{24}{(1 + N) N (1 + N) (2 + N)} S_1 \right] S_{3,1} \\
&+ \frac{2 S_{3,2}}{N + 2} + \left[ -\frac{12 (-1)^N}{(N - 1) N (N + 1) (N + 2)} - \frac{3}{N + 2} \right] S_{4,1} \\
&\frac{2 S_{2,1} S_{2,1}}{2 + N} + \frac{4 S_{3,2} S_{2,1}}{N + 2} + \left[ (-1)^N \frac{2 (6 - 23 N + 9 N^2 + 2 N^3)}{(1 + N) N (1 + N) (2 + N)} \right] S_{2,1,1} - \frac{2 S_{2,1,1,2}}{N + 2} \\
&+ (-1)^N \frac{1}{(1 + N) N (1 + N) (2 + N)} \left[ 42 S_{2,2,1} - 24 S_{3,1,1} + 54 S_{2,1,1,1} \right] \\
&- (-1)^N \frac{30}{(1 + N) N (1 + N) (2 + N)} S_{3,1} \left( \frac{1}{2} \right) \tilde{S}_1 (2) \\
&+ (-1)^N \frac{30}{(1 + N) N (1 + N) (2 + N)} S_1 \tilde{S}_1 \left( \frac{1}{2} \right) \tilde{S}_3 (2) + \left\{ (-1)^N \frac{2 (6 - 12 N + 7 N^2 + N^3)}{(1 + N) N (1 + N) (2 + N)} \right\} \\
&\frac{6 S_1^2}{(1 + N)^2 N^3} + (-1)^N \frac{2 (6 - 23 N + 9 N^2 + 2 N^3)}{(1 + N) N (1 + N) (2 + N)} S_1 \tilde{S}_1 (2) \\
&+ \left[ (-1)^N \frac{2 (6 - 23 N + 9 N^2 + 2 N^3)}{(1 + N) N (1 + N) (2 + N)} + (-1)^N \frac{12}{(1 + N) N (1 + N) (2 + N)} S_1 \right] \tilde{S}_2 (2) \\
&+ \left\{ (-1)^N \frac{12 S_1^2}{(1 + N) N (1 + N) (2 + N)} \right\} \tilde{S}_3 (2) + \left\{ (-1)^N \frac{2 (6 - 12 N + 7 N^2 + N^3)}{(1 + N) N (1 + N) (2 + N)} \right\} \left( \frac{1}{2} \right) \\
&\frac{6}{(1 + N) N (1 + N) (2 + N)} \tilde{S}_3 (2) + \left\{ (-1)^N \frac{2 (6 - 12 N + 7 N^2 + N^3)}{(1 + N) N (1 + N) (2 + N)} \right\} \left( \frac{1}{2} \right) \\
&\frac{2 (6 - 23 N + 9 N^2 + 2 N^3)}{(1 + N)^2 N^2 (1 + N) (2 + N)} S_1 \tilde{S}_1 \left( \frac{1}{2} \right) + (-1)^N \frac{2 (6 - 23 N + 9 N^2 + 2 N^3)}{(1 + N)^2 N^2 (1 + N) (2 + N)} S_1 \tilde{S}_3 (2) + \left\{ (-1)^N \frac{2 (6 - 12 N + 7 N^2 + N^3)}{(1 + N) N (1 + N) (2 + N)} \right\} \left( \frac{1}{2} \right) \\
&\frac{2 (6 - 23 N + 9 N^2 + 2 N^3)}{(1 + N)^2 N^2 (1 + N) (2 + N)} S_1 \\
&\frac{2 (6 - 23 N + 9 N^2 + 2 N^3)}{(1 + N)^2 N^2 (1 + N) (2 + N)} S_1
\end{align*}
\]
\[-\frac{(-1)^N}{(-1 + N)N(1 + N)(2 + N)} \left[ 66S_{1,1,3} \left( \frac{1}{2}, 1, 2 \right) + 36S_{1,1,3} \left( \frac{1}{2}, 2, 1 \right) \right] + 30S_{1,1,3} \left( \frac{1}{2}, 2, 1 \right) + 30S_{1,1,3} \left( 1, 2, \frac{1}{2} \right) \]

\[+ \left( -1 \right)^N \frac{4(6 - 23N + 9N^2 + 2N^3)}{(-1 + N)^2N^2(1 + N)(2 + N)} - \frac{24}{(-1 + N)N(1 + N)(2 + N)} S_1 \]

\[\times \left[ S_{1,2,1} \left( \frac{1}{2}, 2, 1 \right) - S_{1,2,1} \left( 2, \frac{1}{2}, 1 \right) - \frac{1}{2} S_{1,2,1} \left( 2, 1, \frac{1}{2} \right) \right] \]

\[-\frac{(-1)^N}{(-1 + N)N(1 + N)(2 + N)} \left[ 30\tilde{S}_{1,2,2} \left( \frac{1}{2}, 1, 2 \right) + 36\tilde{S}_{1,2,2} \left( \frac{1}{2}, 2, 1 \right) \right] + 48\tilde{S}_{1,3,1} \left( \frac{1}{2}, 2, 1 \right) + 30\tilde{S}_{1,3,1} \left( 1, \frac{1}{2}, 2 \right) + 30\tilde{S}_{1,3,1} \left( 1, 2, \frac{1}{2} \right) + 30\tilde{S}_{1,2,1} \left( \frac{1}{2}, 2, 1 \right) + 30\tilde{S}_{1,2,1} \left( 1, 2, \frac{1}{2} \right) + 30\tilde{S}_{2,1,2} \left( \frac{1}{2}, 2, 1 \right) - 24\tilde{S}_{2,1,2} \left( 2, \frac{1}{2}, 1 \right) - 24\tilde{S}_{2,1,2} \left( 2, 1, \frac{1}{2} \right) + 30\tilde{S}_{3,1,1} \left( \frac{1}{2}, 1, 2 \right) + 30\tilde{S}_{3,1,1} \left( \frac{1}{2}, 2, 1 \right) \]

\[+ \left( -1 \right)^N \frac{2(6 - 23N + 9N^2 + 2N^3)}{(-1 + N)^2N^2(1 + N)(2 + N)} \]

\[+ \left( -1 \right)^N \frac{12}{(-1 + N)N(1 + N)(2 + N)} \left[ \tilde{S}_{1,1,1,1} \left( \frac{1}{2}, 1, 2, 1 \right) \right] \]

\[-2\tilde{S}_{1,1,1,1} \left( 2, \frac{1}{2}, 1, 1 \right) - 2\tilde{S}_{1,1,1,1} \left( 2, 1, \frac{1}{2}, 1 \right) - 2\tilde{S}_{1,1,1,1} \left( 2, 1, 1, \frac{1}{2} \right) \]

\[+ \frac{(-1)^N}{(-1 + N)N(1 + N)(2 + N)} \left[ 66\tilde{S}_{1,1,1,2} \left( \frac{1}{2}, 1, 2, 1 \right) + 48\tilde{S}_{1,1,1,2} \left( \frac{1}{2}, 2, 1, 1 \right) \right] + 30\tilde{S}_{1,1,1,2} \left( \frac{1}{2}, 2, 1, 1 \right) + 30\tilde{S}_{1,1,1,2} \left( 1, 2, \frac{1}{2}, 1 \right) + 30\tilde{S}_{1,1,1,2} \left( \frac{1}{2}, 1, 1, 2 \right) \]

\[+ 12\tilde{S}_{1,1,2,1} \left( \frac{1}{2}, 1, 2, 1 \right) + 48\tilde{S}_{1,1,2,1} \left( \frac{1}{2}, 2, 1, 1 \right) + 30\tilde{S}_{1,1,2,1} \left( \frac{1}{2}, 2, 1, 1 \right) + 30\tilde{S}_{1,1,2,1} \left( \frac{1}{2}, 1, 1, 2 \right) \]

\[+ 30\tilde{S}_{1,1,2,1} \left( 1, 2, 1, \frac{1}{2} \right) + 30\tilde{S}_{1,2,1,1} \left( \frac{1}{2}, 1, 1, 2 \right) + 30\tilde{S}_{1,2,1,1} \left( \frac{1}{2}, 1, 2, 1 \right) \]

\[+ 12\tilde{S}_{1,2,1,1} \left( \frac{1}{2}, 2, 1, 1 \right) + 30\tilde{S}_{1,2,1,1} \left( 1, 1, \frac{1}{2}, 2 \right) + 30\tilde{S}_{1,2,1,1} \left( 1, 1, 2, \frac{1}{2} \right) \]

\[+ 30\tilde{S}_{1,2,1,1} \left( \frac{1}{2}, 1, 2, 1 \right) + 30\tilde{S}_{2,1,1,1} \left( \frac{1}{2}, 2, 1, 1 \right) + 30\tilde{S}_{2,1,1,1} \left( \frac{1}{2}, 1, 1, 2 \right) \]

\[+ 30\tilde{S}_{2,1,1,1} \left( \frac{1}{2}, 1, 2, 1 \right) + 30\tilde{S}_{2,1,1,1} \left( \frac{1}{2}, 1, 2, 1 \right) + 30\tilde{S}_{2,1,1,1} \left( 1, 2, 1, \frac{1}{2} \right) \]
\[-24 \tilde{S}_{2,1,1,1} \left( 2, \frac{1}{2}, 1, 1 \right) - 24 \tilde{S}_{2,1,1,1} \left( 2, 1, \frac{1}{2}, 1 \right) - 24 \tilde{S}_{2,1,1,1} \left( 2, 1, 1, \frac{1}{2} \right) - 12 \tilde{S}_{1,1,1,1,1} \left( \frac{1}{2}, 1, 2, 1, 1 \right) - 36 \tilde{S}_{1,1,1,1,1,1} \left( \frac{1}{2}, 2, 1, 1, 1 \right) \]

\[\begin{aligned}
&+ \left\{ (-1)^N \frac{3 \tilde{S}_1^2}{(-1 + N)N(1 + N)(2 + N)} + (-1)^N \frac{2 + 9N - 5N^2}{(-1 + N)^2N(1 + N)(2 + N)} \\
&+ (-1)^N \frac{6 - 11N + 2N^2}{(-1 + N)^2N^2(2 + N)} S_1 \\
&+ \left[ \frac{3(-1)^N}{(N - 1)N(N + 1)(N + 2)} + \frac{1}{N + 2} \right] S_2 \right\} \zeta_3 \\
&+ \zeta_2 \left\{ (-1)^N \frac{9 \tilde{S}_1^2}{2(-1 + N)N(1 + N)(2 + N)} \\
&+ (-1)^N \frac{2 + 3N - 2^2 + N - 2^2N^2 - 3 \cdot 2^1 + N^2}{(-1 + N)^3N^2(1 + N)(2 + N)} \\
&+ \left\{ (-1)^N \frac{12 - 2^2 + N^2}{2(-1 + N)^2N^2(1 + N)(2 + N)} \\
&+ \left[ \frac{1}{N + 2} + \frac{6(-1)^N}{(N - 1)N(N + 1)(N + 2)} \right] S_1 \\
&+ \frac{1}{N(N + 2)} \right\} S_2 + \left[ \frac{6(-1)^N}{(N - 1)N(N + 1)(N + 2)} - \frac{2}{N + 2} \right] S_3 \\
&- \frac{2S_{-2}}{N(N + 2)} + \left[ (-1)^N \frac{-6 + 3N + 18N^2 - 20N^3 - 3N^4 + 2N^5}{(-1 + N)^3N^3(1 + N)(2 + N)} \\
&+ \frac{2S_{-2}}{N + 2} \right] S_1 + \frac{3S_{-3}}{N + 2} + (-1)^N \frac{12}{(1 + N)N(1 + N)(2 + N)} S_{2,1} \\
&- \frac{2S_{-2,1}}{N + 2} + \left[ (-1)^N \frac{3 \tilde{S}_1^2}{(-1 + N)N(1 + N)(2 + N)} \\
&+ (-1)^N \frac{6 - 12N + 7N^2 + N^3}{(-1 + N)^3N^3} + (-1)^N \frac{-6 + 23N - 9N^2 - 2N^3}{(-1 + N)^2N^2(1 + N)(2 + N)} S_1 \right] \tilde{S}_1(2) \\
&+ \left[ (-1)^N \frac{-6 + 23N - 9N^2 - 2N^3}{(-1 + N)^2N^2(1 + N)(2 + N)} \\
&- (-1)^N \frac{6}{(1 + N)N(1 + N)(2 + N)} \right] \tilde{S}_2(2) \\
&+ \left[ (-1)^N \frac{6 - 23N + 9N^2 + 2N^3}{(-1 + N)^2N^2(1 + N)(2 + N)} \\
&+ (-1)^N \frac{6}{(1 + N)N(1 + N)(2 + N)} S_1 \right] \tilde{S}_{1,1}(2, 1) \\
&- (-1)^N \frac{3}{(1 + N)N(1 + N)(2 + N)} \tilde{S}_3(2) \\
&+ \frac{(-1)^N}{(1 + N)N(1 + N)(2 + N)} \left[ 3 \tilde{S}_{1,2}(2, 1) - 15 \tilde{S}_{2,1}(1, 2) + 6 \tilde{S}_{2,1}(2, 1) - 6 \tilde{S}_{1,1,1}(2, 1, 1) \right] \right\} \]
\[ N^{-2-j+N-2} \sum_{j=1}^{N} \sum_{j_1=1}^{N} \sum_{n=1}^{\infty} (-1)^{j_{1}} j B(j,n) (-j+N-2) S_{1}(j) S_{1}(n) \]
\[ = \sum_{j=1}^{N} \sum_{j_1=1}^{N} \sum_{n=1}^{\infty} \left( \frac{(-1)^{j_{1}} j B(j,n) (-j+N-2) S_{1}(j) S_{1}(n)}{N^{3}(1+N)(2+N)} \right) \]
\[ = \sum_{j=1}^{N} \sum_{j_1=1}^{N} \sum_{n=1}^{\infty} \left( \frac{(-1)^{j_{1}} j B(j,n) (-j+N-2) S_{1}(j) S_{1}(n)}{N^{3}(1+N)(2+N)} \right) \]
\[ = \frac{(-1)^{N} 4}{(1+N)(2+N)} S_{-2} + S_{2} \left\{ \frac{-8 - 2N + N^{2} + 5N^{3} + 5N^{4}}{4N^{3}(1+N)(2+N)} \right\}
\[ + \left[ \frac{(-1)^{N}(N-1)}{N^{2}(2+N)} + \frac{1}{2N^{2}(N+1)} \right] S_{1} + (-1)^{N} \frac{2}{N(2+N)} S_{-2} \]
\[ - \frac{2(-1)^{N}}{(N+1)(N+2)} \right\} \]
\[ + \left[ \frac{(-1)^{N}(1-N)}{N^{2}(2+N)} + \frac{1}{2(N+2)} \right] S_{2,1} - (-1)^{N} \frac{2}{N(2+N)} S_{2,-2} \]
\[ + \left[ \frac{(-1)^{N}}{N(N+2)} + \frac{1}{2(N+2)} \right] S_{3,1} + \left[ (-1)^{N} \frac{2}{N(2+N)} S_{1} \right] \]
\[ = \frac{3(-1)^{N}}{N(2+N)} S_{-4} \]
\[ + \left[ \frac{(-1)^{N}(1-N)}{N^{2}(2+N)} + \frac{1}{2(N+2)} \right] S_{2,1} - (-1)^{N} \frac{2}{N(2+N)} S_{2,-2} \]
\[ + \left[ \frac{(-1)^{N}}{N(N+2)} + \frac{1}{2(N+2)} \right] S_{3,1} + \left[ (-1)^{N} \frac{2}{N(2+N)} S_{1} \right] \]
\[ = \frac{4}{N(2+N)} S_{-2,1,1} \right] + \left[ \frac{16 + 4N - 2N^{2} + N^{3} + N^{4}}{8N^{3}(1+N)(2+N)} \right] - \frac{S_{1}}{2N^{2}(N+1)} \]
\[ + \frac{(-1)^{N}}{N^{3}(N+1)(N+2)} \right]\] 
\[ = \sum_{j=1}^{N} \sum_{j_1=1}^{N} \sum_{n=1}^{\infty} \left( \frac{(-1)^{j_{1}} j B(j,n) (-j+N-2) S_{1}(j) S_{1}(n)}{N^{3}(1+N)(2+N)} \right) \]
\[ = \frac{S_{2}^{2}}{4(N+2)} + \left[ \frac{(-1)^{N} S_{1}^{2}}{2N(N+2)} + \left[ \frac{(-1)^{N}}{N(N+2)} - \frac{1}{2N^{2}(N+1)} \right] \right] S_{1} \]
\[- \frac{N^2 + 1}{2N^2(N + 1)} + (-1)^{N} \left[ \frac{1}{N(2 + N)}S_{-2} + \frac{1}{(N + 1)(N + 2)} \right] S_2 \]
\[+ (-1)^{N} \frac{8 - 19N + 24N^2}{8(-1 + N)N^2(1 + N)(2 + N)} + \frac{-48 - 24N + 71N^2 + 95N^3}{48N^2(1 + N)(2 + N)} \]
\[- \frac{S_3}{2N^2(N + 1)} + \left[ - \frac{(-1)^{N}}{2N(N + 2)} - \frac{1}{4(N + 2)} \right] S_4 \]
\[+ (-1)^{N} \left[ \frac{2}{(1 + N)(2 + N)}S_{-2} + \frac{1}{N(2 + N)}S_1^2S_{-2} + \frac{1}{N(2 + N)}S_{-3} \right] + S_1 \left[ - \frac{2}{N(2 + N)}S_{-2} - \frac{1}{N(2 + N)}S_{-3} \right] \]
\[- \frac{1}{N(2 + N)}S_{-4} \right] + \left[ - (-1)^{N} \frac{1}{N(2 + N)}S_1 + \frac{1}{2N^2(N + 1)} \right] \]
\[\frac{(-1)^{N}}{N(N + 2)} ] S_{-2,1} \]
\[+ (-1)^{N} \left[ \frac{1}{N(2 + N)}S_{-3,1} + \frac{1}{N(2 + N)}S_{2,1,1} + \frac{2}{N(2 + N)}S_{-2,1,1} \right] \]
\[+ \left[ \frac{-2 + N - 2N^2}{2(-1 + N)N^2(1 + N)(2 + N)} + \frac{2 + N - N^2 - 2N^3}{2N^2(1 + N)(2 + N)} + \frac{S_1}{2N^2(N + 1)} \right] \]
\[+ \left[ \frac{1}{2(N + 2)} - \frac{(-1)^{N}}{N(N + 2)} \right] S_2 + \left[ \frac{(-1)^{N}}{N(2 + N)}S_{-2} \right] \zeta_2 \]
\[+ \left[ \frac{-12 - 6N + N^2 + N^3}{12N^2(1 + N)(2 + N)} + \frac{(-1)^{N}}{(N - 1)N^2(N + 1)(N + 2)} \right] S_{-2} \]
\[\sum_{j=1}^{N^2} \sum_{j_1=1}^{N^2-j} (-1)^{j} (-1)^{j_1} \left( \frac{S_1(j)S_2(-j_1 + N)}{(j + 2)(j_1 - N - 2)} \right) = \]
\[\left[ \frac{(-1)^{N}}{2(N + 1)(N + 2)} \right] S_2 + \left[ \frac{S_1^2}{2(N + 2)} \right] \]
\[+ \left[ \frac{-3 - 3N - N^2}{(1 + N)^2(2 + N)^2} + (-1)^{N} \frac{-4 - 5N - 3N^2 - N^3}{N(1 + N)^2(2 + N)^2} \right] S_1 \]
\[+ (-1)^{N} \frac{8 + 28N + 37N^2 - 42N^4 - 38N^5 - 14N^6 - 2N^7}{2N^2(1 + N)^3(2 + N)^3} \]
\[+ \frac{8 + 28N + 49N^2 + 39N^3 + 6N^4 - 10N^5 - 6N^6 - N^7}{N^2(1 + N)^3(2 + N)^3} \]
\[+ (-1)^{N} \left[ \frac{-2}{(1 + N)(2 + N)} + \frac{(-8 - 28N - 27N^2 - 8N^3)S_1^2}{2N^2(1 + N)^3(2 + N)^3} \right] \]
\[+ \frac{4 + 5N + 3N^2 + N^3}{N(1 + N)^3(2 + N)^2} + \left[ \frac{(-8 - 28N - 8N^2 - 6N^3 - N^4)}{(1 + N)^3(2 + N)^3} \right] \]

\[(G.5)\]
\begin{align}
\pm (-1)^N \left[ -4 - 3N + 2N^2 + 3N^3 + N^4 \frac{1}{N(1+N)^2(2+N)^2} + \frac{1}{(1+N)(2+N)} S_1 \right] S_3 \\
\pm (-1)^N \left[ \frac{3}{2(1+N)(2+N)} S_4 - \frac{2(-4 + 2N^2 + N^3)}{N^2(2+N)^2} S_{-2} \right] + S_1 \left[ (-1)^N \frac{16 + 8N - 4N^2 - N^3}{N^3(2+N)^3} \right] + S_2 \left[ (-1)^N \frac{3}{(1+N)(2+N)} S_{-3} \right] \\
\pm \left[ \frac{1}{(N+1)^2(N+2)} \right] + (-1)^N \left[ + \frac{2}{(1+N)(2+N)} S_{-4} + \frac{4}{(1+N)(2+N)} S_{2,-2} \right] \\
\pm \left[ - \frac{2(-4 - 3N + 2N^2 + 3N^3 + N^4)}{N(1+N)^2(2+N)^2} - \frac{2}{(1+N)(2+N)} S_1 \right] S_{-2,1} \\
\pm \left[ \frac{6}{(1+N)(2+N)} S_{-3,1} + \frac{4}{(1+N)(2+N)} S_{-2,1,1} \right] \end{align}

(G.6)

The nested sums emerging in this work, which were not given before in Refs. [120, 121] and those being closer related to the structure of harmonic sums [125], are of the type illustrated above. The latter have been calculated using C. Schneider’s packages Sigma [140–143], EvaluateInfiniteSums [239] and J. Ablinger’s package HarmonicSums [202, 240]. The involved structure of Eq. (G.3) requires simplifications due to explicit algebraic and structural relations for the generalized harmonic sums. These will be given in an upcoming publication Ref. [206].
H Fixed Moments

H.1 3-loop Moments to the anomalous dimensions

In the following we list the $O(T_F^2 n_f C_{F,A})$ contributions to the fixed moments of the anomalous dimensions related to the present calculation. We have used them for comparison in recalculating the corresponding contributions to the anomalous dimensions at general values of $N$, cf. Eqs. (194,210,218).

(i) $\hat{\gamma}^{(2)}_{qq}$ :

\[
\hat{\gamma}^{(2)}_{qq}(2) = T_F^2 n_f \left( \frac{16928}{243} C_A - \frac{2768}{243} C_F \right)
\]

(H.1)

\[
\hat{\gamma}^{(2)}_{qq}(4) = T_F^2 n_f \left( \frac{4481539}{151875} C_A + \frac{9613841}{151875} C_F \right)
\]

(H.2)

\[
\hat{\gamma}^{(2)}_{qq}(6) = T_F^2 n_f \left( \frac{86617163}{5834430} C_A + \frac{1539874183}{170170875} C_F \right)
\]

(H.3)

\[
\hat{\gamma}^{(2)}_{qq}(8) = T_F^2 n_f \left( \frac{10379424541}{1377810000} C_A + \frac{79032978461}{81015228000} C_F \right)
\]

(H.4)

\[
\hat{\gamma}^{(2)}_{qq}(10) = T_F^2 n_f \left( \frac{1669885489}{494133750} C_A + \frac{1584713325754369}{1618003904375} C_F \right)
\]

(H.5)

(ii) $\hat{\gamma}^{(2),PS}_{qq}$ :

\[
\hat{\gamma}^{(2),PS}_{qq}(2) = -T_F^2 n_f C_F \frac{10048}{243}
\]

(H.6)

\[
\hat{\gamma}^{(2),PS}_{qq}(4) = -T_F^2 n_f C_F \frac{123734}{151875}
\]

(H.7)

\[
\hat{\gamma}^{(2),PS}_{qq}(6) = -T_F^2 n_f C_F \frac{252446104}{72930375}
\]

(H.8)

\[
\hat{\gamma}^{(2),PS}_{qq}(8) = -T_F^2 n_f C_F \frac{13131081443}{6751269000}
\]

(H.9)

\[
\hat{\gamma}^{(2),PS}_{qq}(10) = -T_F^2 n_f C_F \frac{531694610144}{420260754375}
\]

(H.10)

\[
\hat{\gamma}^{(2),PS}_{qq}(12) = -T_F^2 n_f C_F \frac{2566080055386457}{2851637832143100}
\]

(H.11)

(iii) $\hat{\gamma}^{(2),NS,+}_{qq}$ :

\[
\hat{\gamma}^{(2),NS,+}_{qq}(2) = -T_F^2 n_f C_F \frac{3584}{243}
\]

(H.13)
\( \hat{\gamma}_{qq}^{(2),\text{NS},+} (4) = -T_F^2 n_f C_F \frac{768554}{30375} \)  \( \text{(H.14)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},+} (6) = -T_F^2 n_f C_F \frac{321390284}{10418625} \)  \( \text{(H.15)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},+} (8) = -T_F^2 n_f C_F \frac{3892097797}{1125211500} \)  \( \text{(H.16)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},+} (10) = -T_F^2 n_f C_F \frac{2799590105687}{748828253250} \)  \( \text{(H.17)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},+} (12) = -T_F^2 n_f C_F \frac{651585338758071}{1645175672390250} \)  \( \text{(H.18)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},+} (14) = -T_F^2 n_f C_F \frac{6816716625776019}{1645175672390250} \)  \( \text{(H.19)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},-} (1) = 0 \)  \( \text{(H.21)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},-} (3) = -T_F^2 n_f C_F \frac{5138}{243} \)  \( \text{(H.22)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},-} (5) = -T_F^2 n_f C_F \frac{862484}{30375} \)  \( \text{(H.23)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},-} (7) = -T_F^2 n_f C_F \frac{1369936511}{41674500} \)  \( \text{(H.24)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},-} (9) = -T_F^2 n_f C_F \frac{20297329837}{562605750} \)  \( \text{(H.25)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},-} (11) = -T_F^2 n_f C_F \frac{28869611542843}{748828253250} \)  \( \text{(H.26)} \)

\( \hat{\gamma}_{qq}^{(2),\text{NS},-} (13) = -T_F^2 n_f C_F \frac{66727681292862571}{1645175672390250} \)  \( \text{(H.27)} \)
H.2 The $O(\varepsilon^0)$ Contributions to $\hat{A}^{(3)}_{ij}$

We list the contributions $O(T^2 n_f C_{F,A})$ to the fixed moments of the constant part of the unrenormalized massive OMEs, $\hat{a}_{ij}^{(3,K)}$ from Ref. [95]. We used these values for comparisons to the general $N$-results computed in the present paper, Eqs. (176,200,206,215).

\[ v \] $a_{Qg}^{(3)}$

\[ a_{Qg}^{(3)}(2) = n_f T_F^2 C_A \left( \frac{6706}{2187} - \frac{616}{81} \zeta_3 - \frac{250}{81} \zeta_2 \right) + T_F^2 n_F C_F \left( \frac{158}{243} + \frac{896}{81} \zeta_3 + \frac{40}{9} \zeta_2 \right), \]  
\[ a_{Qg}^{(3)}(4) = n_f T_F^2 C_A \left( \frac{947836283}{72900000} - \frac{18172}{2025} \zeta_3 - \frac{11369}{13500} \zeta_2 \right) + T_F^2 n_F C_F \left( \frac{8164734347}{4374000000} + \frac{130207}{20250} \zeta_3 + \frac{1694939}{810000} \zeta_2 \right), \]  
\[ a_{Qg}^{(3)}(6) = n_f T_F^2 C_A \left( \frac{12648331693}{735138180} - \frac{4433}{567} \zeta_3 + \frac{23311}{111132} \zeta_2 \right) + T_F^2 n_F C_F \left( \frac{8963002169173}{1715322420000} + \frac{111848}{19845} \zeta_3 + \frac{11873563}{19448100} \zeta_2 \right), \]  
\[ a_{Qg}^{(3)}(8) = n_f T_F^2 C_A \left( \frac{24718362393463}{1326976600000} - \frac{125356}{18225} \zeta_3 + \frac{2118187}{2916000} \zeta_2 \right) + T_F^2 n_F C_F \left( -\frac{291376419801571603}{32665339929600000} + \frac{887741}{174960} \zeta_3 - \frac{49652772817}{93391278750} \zeta_2 \right), \]  
\[ a_{Qg}^{(3)}(10) = n_f T_F^2 C_A \left( \frac{297277185134077151}{15532837481700000} - \frac{1505896}{245025} \zeta_3 \right) + T_F^2 n_F C_F \left( -\frac{1178560772273339822317}{107642563748181000000} \right), \]  
\[ + \frac{189965849}{188669250} \zeta_2 \right), + T_F^2 n_F C_F \left( -\frac{1178560772273339822317}{107642563748181000000} \right), \]  
\[ + \frac{62292104}{13476375} \zeta_3 - \frac{49652772817}{93391278750} \zeta_2 \right). \]  
\[ \text{(H.28)} \]
(vi) $a_{Qq}^{(3),PS}$:

$$
a_{Qq}^{(3),PS} \, (2) = T^2 n_F C_F \left( -\frac{76408}{2187} + \frac{896}{81} \zeta_3 - \frac{112}{81} \zeta_2 \right), \quad \text{(H.33)}
$$

$$
a_{Qq}^{(3),PS} \, (4) = T^2 n_F C_F \left( -\frac{474827503}{109350000} + \frac{3388}{2025} \zeta_3 - \frac{851}{20250} \zeta_2 \right), \quad \text{(H.34)}
$$

$$
a_{Qq}^{(3),PS} \, (6) = T^2 n_F C_F \left( -\frac{82616977}{45378900} + \frac{1936}{2835} \zeta_3 - \frac{16778}{694575} \zeta_2 \right), \quad \text{(H.35)}
$$

$$
a_{Qq}^{(3),PS} \, (8) = T^2 n_F C_F \left( -\frac{16194572439593}{1512284256000} + \frac{1369}{3645} \zeta_3 - \frac{343781}{14288400} \zeta_2 \right), \quad \text{(H.36)}
$$

$$
da_{Qq}^{(3),PS} \, (10) = T^2 n_F C_F \left( -\frac{454721266324013}{624087220246875} + \frac{175616}{735075} \zeta_3 - \frac{547424}{24257475} \zeta_2 \right), \quad \text{(H.37)}
$$

$$
da_{Qq}^{(3),PS} \, (12) = T^2 n_F C_F \left( -\frac{6621557709293056160177}{12331394510293050192000} + \frac{24964}{150579} \zeta_3 - \frac{1291174013}{63306423180} \zeta_2 \right). \quad \text{(H.38)}
$$

(vii) $a_{qq,Q}^{(3),PS}$:

$$
a_{qq,Q}^{(3),PS} \, (2) = n_f T^2 C_F \left( -\frac{100096}{2187} + \frac{896}{81} \zeta_3 - \frac{256}{81} \zeta_2 \right), \quad \text{(H.39)}
$$

$$
a_{qq,Q}^{(3),PS} \, (4) = n_f T^2 C_F \left( -\frac{118992563}{21870000} + \frac{3388}{2025} \zeta_3 - \frac{4739}{20250} \zeta_2 \right), \quad \text{(H.40)}
$$

$$
a_{qq,Q}^{(3),PS} \, (6) = n_f T^2 C_F \left( -\frac{17732294117}{10210252500} + \frac{1936}{2835} \zeta_3 - \frac{9794}{694575} \zeta_2 \right), \quad \text{(H.41)}
$$

$$
a_{qq,Q}^{(3),PS} \, (8) = n_f T^2 C_F \left( -\frac{20110404913057}{2722116608000} + \frac{1369}{3645} \zeta_3 + \frac{135077}{4762800} \zeta_2 \right), \quad \text{(H.42)}
$$

$$
a_{qq,Q}^{(3),PS} \, (10) = n_f T^2 C_F \left( -\frac{308802524517334}{873722108345625} + \frac{175616}{735075} \zeta_3 + \frac{4492016}{121287375} \zeta_2 \right), \quad \text{(H.43)}
$$

$$
a_{qq,Q}^{(3),PS} \, (12) = n_f T^2 C_F \left( -\frac{6724380501633998071}{38535607844665781850} + \frac{24964}{150579} \zeta_3 + \frac{583767694}{15826605795} \zeta_2 \right), \quad \text{(H.44)}
$$
\[ a_{qq,Q}^{(3),PS} (14) = n_f T_F^2 C_F \left( -\frac{616164615443256347333}{754543370385064260000} + \frac{22472}{184275} \zeta_3 + \frac{189601441}{5533778250} \zeta_2 \right). \] 

(H.45)

\((viii) \ a_{qq,Q}^{(3),NS} :\)

\[ a_{qq,Q}^{(3),NS} (1) = 0 , \] 

(H.46)

\[ a_{qq,Q}^{(3),NS} (2) = T_F^2 n_F C_F \left( -\frac{100096}{2187} + \frac{896}{81} \zeta_3 - \frac{256}{81} \zeta_2 \right), \] 

(H.47)

\[ a_{qq,Q}^{(3),NS} (3) = T_F^2 n_F C_F \left( -\frac{1271507}{17496} + \frac{1400}{81} \zeta_3 - \frac{415}{81} \zeta_2 \right), \] 

(H.48)

\[ a_{qq,Q}^{(3),NS} (4) = T_F^2 n_F C_F \left( -\frac{1006358899}{10935000} + \frac{8792}{405} \zeta_3 - \frac{13271}{2025} \zeta_2 \right), \] 

(H.49)

\[ a_{qq,Q}^{(3),NS} (5) = T_F^2 n_F C_F \left( -\frac{195474809}{1822500} + \frac{10192}{405} \zeta_3 - \frac{15566}{2025} \zeta_2 \right), \] 

(H.50)

\[ a_{qq,Q}^{(3),NS} (6) = T_F^2 n_F C_F \left( -\frac{524427335513}{4375822500} + \frac{11344}{405} \zeta_3 - \frac{856238}{99225} \zeta_2 \right), \] 

(H.51)

\[ a_{qq,Q}^{(3),NS} (7) = T_F^2 n_F C_F \left( -\frac{54861581223623}{420078960000} + \frac{4108}{135} \zeta_3 - \frac{3745727}{396900} \zeta_2 \right), \] 

(H.52)

\[ a_{qq,Q}^{(3),NS} (8) = T_F^2 n_F C_F \left( -\frac{4763338626853463}{34026395760000} + \frac{39532}{1215} \zeta_3 - \frac{36241943}{3572100} \zeta_2 \right), \] 

(H.53)

\[ a_{qq,Q}^{(3),NS} (9) = T_F^2 n_F C_F \left( -\frac{2523586499054071}{17013197880000} + \frac{8360}{243} \zeta_3 - \frac{19247947}{1786050} \zeta_2 \right), \] 

(H.54)

\[ a_{qq,Q}^{(3),NS} (10) = T_F^2 n_F C_F \left( -\frac{38817494524177585991}{249090230161080000} + \frac{96440}{2673} \zeta_3 - \frac{2451995507}{216112050} \zeta_2 \right), \] 

(H.55)

\[ a_{qq,Q}^{(3),NS} (11) = T_F^2 n_F C_F \left( -\frac{40517373495580091423}{249090230161080000} + \frac{50252}{13365} \zeta_3 - \frac{512808781}{43222410} \zeta_2 \right), \] 

(H.56)
\[ a_{qq,Q}^{(3),\text{NS}} (12) = T_F^2 n_F C_F \left( -\frac{1201733391177720469772303}{714266063630605880000} + \frac{6774784}{173745} \zeta_3 
- \frac{90143221429}{7304587290} \zeta_2 \right), \tag{H.57} \]

\[ a_{qq,Q}^{(3),\text{NS}} (13) = T_F^2 n_F C_F \left( -\frac{1242840812874342588467303}{714266063630605880000} + \frac{6997864}{173745} \zeta_3 
- \frac{93360116539}{7304587290} \zeta_2 \right), \tag{H.58} \]

\[ a_{qq,Q}^{(3),\text{NS}} (14) = T_F^2 n_F C_F \left( -\frac{256205552272074402170491}{1422853212726121176000} + \frac{1440968}{34749} \zeta_3 
- \frac{481761665447}{36522936450} \zeta_2 \right). \tag{H.60} \]
H.3 3–loop Moments for Transversity

We list below the contributions $O(T_F^2 n_f C_{F,A})$ to the fixed moments of the transversity anomalous dimension, cf. [179], to which we compared the result for general values of $N$ calculated in the present paper, Eqs. (222), cf. also [203].

\[
\gamma_{qq}^{(2),NS,TR}(1) = -\frac{16}{3} T_F^2 n_f C_F \tag{H.61}
\]
\[
\gamma_{qq}^{(2),NS,TR}(2) = -\frac{368}{27} T_F^2 n_f C_F \tag{H.62}
\]
\[
\gamma_{qq}^{(2),NS,TR}(3) = -\frac{4816}{243} T_F^2 n_f C_F \tag{H.63}
\]
\[
\gamma_{qq}^{(2),NS,TR}(4) = -\frac{29444}{1215} T_F^2 n_f C_F \tag{H.64}
\]
\[
\gamma_{qq}^{(2),NS,TR}(5) = -\frac{837188}{837188} T_F^2 n_f C_F \tag{H.65}
\]
\[
\gamma_{qq}^{(2),NS,TR}(6) = -\frac{6419516}{6419516} T_F^2 n_f C_F \tag{H.66}
\]
\[
\gamma_{qq}^{(2),NS,TR}(7) = -\frac{337002284}{337002284} T_F^2 n_f C_F \tag{H.67}
\]
\[
\gamma_{qq}^{(2),NS,TR}(8) = -\frac{20837250}{20837250} T_F^2 n_f C_F \tag{H.68}
\]
\[
\gamma_{qq}^{(2),NS,TR}(9) = -\frac{562605750}{562605750} T_F^2 n_f C_F \tag{H.69}
\]
\[
\gamma_{qq}^{(2),NS,TR}(10) = -\frac{6188663250}{6188663250} T_F^2 n_f C_F \tag{H.70}
\]
\[
\gamma_{qq}^{(2),NS,TR}(11) = -\frac{748828253250}{748828253250} T_F^2 n_f C_F \tag{H.71}
\]
\[
\gamma_{qq}^{(2),NS,TR}(12) = -\frac{383379490933459}{383379490933459} T_F^2 n_f C_F \tag{H.72}
\]
\[
\gamma_{qq}^{(2),NS,TR}(13) = -\frac{1645175672390250}{1645175672390250} T_F^2 n_f C_F \tag{H.73}
\]

Here we list the $O(T_F^2 n_f C_{F,A})$ moments of the constant part of the unrenormalized massive OMEs $a_{qq,Q}^{(3),TR}$ from Ref. [179]. We used these values for comparisons to the general $N$-result computed in the present paper, Eq. (221).

\[
a_{qq,Q}^{(3),TR}(1) = T_F^2 n_f C_F \left(-\frac{15850}{729} + \frac{112}{27} \zeta_3 - \frac{52}{27} \zeta_2 \right) \tag{H.74}
\]
\[
a_{qq,Q}^{(3),TR}(2) = T_F^2 n_f C_F \left(-\frac{4390}{81} + \frac{112}{9} \zeta_3 - 4 \zeta_2 \right) \tag{H.75}
\]
\[
a_{qq,Q}^{(3),TR}(3) = T_F^2 n_f C_F \left(-\frac{168704}{2187} + \frac{1456}{81} \zeta_3 - \frac{452}{81} \zeta_2 \right) \tag{H.76}
\]
\begin{align*}
\tilde{a}_{qq, Q}^{(3), \text{TR}}(4) &= T^n_F C_F \left( -\frac{20731907}{218700} + \frac{1792}{81} \zeta_3 - \frac{554}{81} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(5) &= T^n_F C_F \left( -\frac{596707139}{5467500} + \frac{10304}{405} \zeta_3 - \frac{15962}{2025} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(6) &= T^n_F C_F \left( -\frac{32472719011}{267907500} + \frac{3808}{135} \zeta_3 - \frac{17762}{2025} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(7) &= T^n_F C_F \left( -\frac{1727972700289}{13127467500} + \frac{1376}{45} \zeta_3 - \frac{947138}{99225} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(8) &= T^n_F C_F \left( -\frac{29573247248999}{210039480000} + \frac{4408}{135} \zeta_3 - \frac{2030251}{198450} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(9) &= T^n_F C_F \left( -\frac{2534665670688119}{17013197880000} + \frac{41912}{1215} \zeta_3 - \frac{19369859}{1786050} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(10) &= T^n_F C_F \left( -\frac{32190808339769663}{2058596943480000} + \frac{43928}{1215} \zeta_3 \\
&\quad - \frac{4072951}{357210} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(11) &= T^n_F C_F \left( -\frac{40628987857774916423}{249090230161080000} + \frac{503368}{13365} \zeta_3 \\
&\quad - \frac{514841791}{43222410} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(12) &= T^n_F C_F \left( -\frac{712685031281296825487}{42096248897222520000} \\
&\quad + \frac{521848}{13365} \zeta_3 - \frac{535118971}{43222410} \zeta_2 \right), \\
\tilde{a}_{qq, Q}^{(3), \text{TR}}(13) &= T^n_F C_F \left( -\frac{1245167831299024242467303}{7114266063630605880000} \\
&\quad + \frac{7005784}{173745} \zeta_3 - \frac{93611152819}{7304587290} \zeta_2 \right).
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Selbstständigkeitserklärung

Hiermit erkläre ich, dass ich diese Arbeit im Rahmen der Betreuung am Deutschen Elektronen-Synchrotron in Zeuthen ohne unzulässige Hilfe Dritter verfasst und alle Quellen als solche gekennzeichnet habe.

Fabian Wißbrock, Berlin den 31. Mai 2010.