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# Massive Two- and Three-loop Calculations in QED and QCD

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## Abstract

This thesis is devoted to the study of mass effects in higher order radiative corrections within QED and QCD. The first part of the thesis deals with the process of deep-inelastic scattering. We compute the full mass dependence of the pure singlet Wilson coefficient in the polarized and unpolarized case to  $\mathcal{O}(\alpha_s^2)$  using iterated integrals over square root valued letters. Through explicit expansion in the limit  $Q^2 \gg m^2$  we prove the factorization of the heavy Wilson coefficient into massless Wilson coefficient and massive operator matrix element in the asymptotic limit. We also derive the first two additional power suppressed coefficients in the expansion. We then turn to the calculation of massive operator matrix elements with two masses. After correcting some inconsistencies of their renormalization in the literature, we extend the variable flavor number scheme to treat the simultaneous decoupling of charm and bottom quarks at next-to-leading order. We also compute missing two-mass contributions to unpolarized operator matrix elements at next-to-next-to-leading order. Afterwards, we extend the calculation to polarized operator matrix elements at next-to-leading and next-to-next-to-leading order in the single and two-mass case. In the case of polarized scattering the calculations at next-to-next-to-leading order provide the first independent check on parts of the polarized anomalous dimensions of Quantum Chromodynamics at this order. For the calculation of these processes we set up new calculational methods, which are introduced together with the calculations.

In the second part of the thesis we deal with QED initial state radiation to electron-positron annihilation into a neutral vector boson at  $\mathcal{O}(\alpha^2)$ . In the literature two independent calculations exist. One is based on explicit phase space integration in the limit that the centre-of-mass energy is much smaller than the electron mass ( $m^2 \ll s$ ) and the other uses factorization in this limit. The two results do not agree. Our calculation, which is based on an exact integration of the phase space and a subsequent expansion, finds agreement with the method based on factorization and thereby proves the factorization of massive external particles in the asymptotic limit for this process. The results derived in this thesis can be used for a more precise description of the above mentioned scattering processes and determination of fundamental parameters of the Standard Model which serve as input for experiments like the LHC. Furthermore, the correction of the  $\mathcal{O}(\alpha^2)$  QED initial state radiation is an important prerequisite for the precision physics at planned  $e^+ e^-$  colliders like the ILC or the FCC<sub>ee</sub>.

## Zusammenfassung

Die Dissertation beschäftigt sich mit dem Einfluss von Massen auf radiative Korrekturen in höherer Ordnung der Störungstheorie. Der erste Teil der Arbeit befasst sich mit der tief-inelastischen Streuung. Wir berechnen die exakte Massenabhängigkeit des *pure singlet* Wilson Koeffizienten im polarisierten und unpolarisierten Fall zu  $\mathcal{O}(\alpha_s^2)$  unter Benutzung von iterierten Integralen mit wurzelwertigen Buchstaben. Durch explizite Entwicklung dieser Objekte im Grenzfall  $Q^2 \gg m^2$  beweisen wir die Faktorisierung dieses Wilson Koeffizienten in den masselosen Wilson Koeffizienten und das massive Operatormatrixelement im asymptotischen Fall. Wir berechnen zusätzlich zwei weitere Ordnungen in der Entwicklung von Potenzkorrekturen. Als nächstes wenden wir uns massiven Operatormatrixelementen im zweimassigen Fall zu. Nachdem wir einige Inkonsistenzen der Renormierung dieser Objekte in der Literatur berichtigen, erweitern wir das *variable flavor number scheme* auf die simultane Entkopplung des *charm* und des *bottom* Quarks auf 2-Schleifen Ordnung. Wir berechnen außerdem noch fehlende zweimassige Korrekturen zu unpolarisierten Operatormatrixelementen auf 3-Schleifen Ordnung. Im Anschluß erfolgt die Berechnung von ausgewählten polarisierten Operatormatrixelementen auf 2- und 3-Schleifen Ordnung. Die Berechnung der polarisierten Operatormatrixelemente auf 3-Schleifen Ordnung stellt die erste unabhängige Verifikation von Teilen der anomalen Dimensionen der Quantenchromodynamik in dieser Ordnung dar. Zur Berechnung dieser radiativen Korrekturen wurden neue Berechnungsmethoden geschaffen, welche in der Dissertation vorgestellt werden.

Der zweite Teil der Arbeit befasst sich mit der QED *initial state radiation* bei der Annihilation eines Elektron-Positron Paares in ein virtuelles und neutrales Vektorboson auf  $\mathcal{O}(\alpha^2)$ . In der Literatur existieren zwei unabhängige Berechnungen. Die erste basiert auf der Berechnung der Phasenraumintegrale im asymptotischen Grenzfall  $m^2 \ll s$ , die zweite auf der Faktorisierung in masselose Streuquerschnitte und massive Operatormatrixelemente in diesem Grenzfall. Die beiden Ergebnisse stimmen nicht überein. Unsere Ergebnisse, welche auf der exakten Phasenraumintegration und einer anschließenden Entwicklung beruhen, finden Übereinstimmung mit den Ergebnissen der zweiten Berechnung und beweisen die Faktorisierung massiver Teilchen in diesem Prozess. Die Ergebnisse dieser Arbeit können für die präzisere Beschreibung von den oben genannten Streuprozessen und einer präziseren Bestimmung elementarer Konstanten des Standardmodells benutzt werden, welche für die genaue experimentelle Auswertung zum Beispiel der Daten des LHC essentiell sind. Mit der Berichtigung der QED *initial state radiation* auf  $\mathcal{O}(\alpha^2)$  wird außerdem eine wichtige Voraussetzung für die Präzisionsphysik an geplanten  $e^+ e^-$  Collidern, wie dem ILC oder dem FCC<sub>ee</sub>, geschaffen.

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# List of Publications

Parts of this thesis have already been published in the following articles:

## Journal Publications

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## Proceedings

J. Ablinger, J. Blümlein, A. De Freitas, A. Goedicke, C. Schneider, K. Schönwald, and F. Wißbrock, “The massive 3-loop operator matrix elements with two masses and the generalized variable flavor number scheme”, PoS (RADCOR2017), 071, arXiv:1712.00745 [hep-ph].

J. Ablinger, J. Blümlein, A. De Freitas, A. Goedicke, C. Schneider, and K. Schönwald, “Two-mass three-loop effects in deep-inelastic scattering”, PoS (LL2018), 051, arXiv:1807.07855 [hep-ph].

## Preprints

J. Blümlein, A. De Freitas, C. Schneider, and K. Schönwald, “The Three Loop Two-Mass Contribution to the Gluon Vacuum Polarization”, arXiv:1710.04500 [hep-ph], unpublished.





# 1. Introduction

Scattering experiments have played a crucial role in understanding the elementary building blocks of nature. One of the first, conducted by Rutherford, Geiger and Madsen, scattered  $\alpha$  particles from a thin gold foil [10–13]. By comparing their results with theoretical predictions from different models it became clear that atoms must consist out of a small positively charged nucleus surrounded by negatively charged electrons [14]. We now know that the nucleus consists out of two different nucleons, the positively charged protons discovered by Rutherford in 1919 [15] and the electrically uncharged neutrons discovered by Chadwick in 1932 [16]. When the anomalous magnetic moments of neutrons and protons were measured and deviated from the ones predicted for point like particles [17–19], a first hint that the nucleons possess substructure was discovered. Later, this was further supported by scattering experiment conducted by Hofstadter which showed extended charge distributions of the nucleons [20–24].

The road to a more fundamental understanding of the substructure began in the 1960s. By then, a large number of hadrons had been detected in cosmic ray and accelerator experiments and a systematic classification of these hadrons was needed. This was achieved by Gell-Mann [25] and Zweig [26] in 1964, when they proposed the quark model. The model introduced three flavors of fractionally charged spin 1/2 fermions, the up ( $u$ ), down ( $d$ ) and strange ( $s$ ) quark. They were able to describe all, at the time, detected hadrons as either a bound state of three quarks (spin 1/2 and 3/2 baryons) or bound states of a quark-antiquark pair (spin 0 and 1 mesons). By assuming an approximate  $SU(3)_{\text{flavor}}$  symmetry between the flavors ('the eightfold way' [27]) it was possible to derive formulas for the masses of the hadrons. An important milestone for this theory was the prediction of the mass of the  $\Omega^-$  baryon before it was experimentally observed [28]. At the same time Gursev and Radicati enlarged the symmetry to a  $SU(6) = SU(2)_{\text{spin}} \otimes SU(3)_{\text{flavor}}$  by introducing spin [29]. This not only unified the mass formulae for baryons and mesons but also enabled them to calculate the ratio of the magnetic moment of the proton and neutron with good agreement with the experiments [30, 31]. Despite all of this success the theory had one major problem. It predicted that the wave functions of the baryons with three quarks of the same flavor, i.e. the  $\Omega^-(sss)$ ,  $\Delta^{++}(uuu)$  and the  $\Delta^-(ddd)$ , to be symmetric, which contradicts the well established spin-statistics theorem [32]. This tension was overcome by Greenberg [33]. His model assigns a three-valued charge, called color, to the quarks which is expressed in terms of para-Fermi statistics. Our current understanding was formed when Nambu [34] and Han and Nambu [35] introduced a new symmetry  $SU(3)_{\text{color}}$  which makes the three-valued charge degree explicit but is completely equivalent to Greenberg's description. Since no color charge was measured at long distances in the experiments the assumption that all particles have to be color neutral was established empirically.

With the advances of technology in the late 1960s it was possible to study the internal structure of the proton at the Stanford Linear Accelerator Center (SLAC) [36–42] by scattering high energetic electrons off of a liquid hydrogen target. For low momentum transfers the cross section shows several peaks corresponding to hadronic resonances and elastic scattering. It was also possible to measure at large energy transfers  $Q^2 > 2 \text{ GeV}^2$ . Here the continuum contribution of deep-inelastic scattering (DIS) is reached. The cross-section can in general be parameterized by several nucleon structure functions  $F_i$  which correspond to the contributing Lorentz structures. The experiments conducted by the SLAC-MIT groups showed that the structure functions which in general depend on the energy transfer  $\nu$  and the momentum transfer  $q^2 = -Q^2$ , from the initial state lepton to the nucleon in its rest frame, only depended on the ratio of  $Q^2$  and  $\nu$ , i.e.  $F_i(\nu, Q^2) = F_i(Q^2/\nu)$ . This behavior was

## 1. Introduction

called scaling and had previously been predicted by Bjorken [43]. His approach was based on current algebra and showed that in the limit  $Q^2 \rightarrow \infty$  and  $\nu \rightarrow \infty$  where the ratio  $Q^2/\nu$  is held fixed, now known as the Bjorken limit, the only relevant parameter is the Bjorken variable  $x = Q^2/2M\nu$  with  $M$  the nucleon's mass. After the experimental discovery of scaling Feynman gave a phenomenological explanation of this behavior of the structure functions in the parton model [44–46]. This model was based on the assumption that the proton is made up out of several point-like constituents, called partons. During the interaction time, which gets shorter and shorter with increasing  $Q^2$ , these partons interact as free particles and the electrons can scatter off of them elastically. The cross-section is therefore given by the incoherent sum of the cross-sections of the partons with the high-energetic lepton weighted by universal parton distribution functions (PDFs)  $f_i(x_i)$ . These parton distributions describe the probabilities to find a given parton  $i$  carrying the fraction  $x_i$  of the total nucleon momentum  $P$  inside the nucleon. Information about the spin of the partons can be extracted from the ratio of the scattering cross section for longitudinally (L) and transversely (T) polarized photons with the nucleon  $R = \sigma_T/\sigma_L$  which can be related to the structure functions  $F_i$  of deep-inelastic scattering. For example spin 0 partons would predict a large  $R$  ratio while for spin 1/2 the ratio is predicted to be small. In the strict parton model the Callan-Gross relation  $R = 0$  [47] holds. While in the beginning the data were not precise enough to measure individual structure functions, later measurements showed that  $R$  is indeed small [37]. This observation supported the hypothesis of point-like spin 1/2 constituents of the proton and ruled out other approaches such as the algebra of fields [48] or vector-meson dominance [49, 50]. The group theoretic approach, which successfully described the nuclear resonances, and the parton model were finally linked by Bjorken and Paschos by identifying quarks with partons [51].

Driven by the success of Quantum Electrodynamics and the unification to the electroweak  $SU(2)_L \times U_Y(1)$  theory proposed by Weinberg in 1967 [52], which build on earlier work of Glashow [53] and Salam and Ward for the leptonic sector [54], one is finally lead to the theory of Quantum Chromodynamics (QCD). In this context Yang-Mills theories, first studied by C.N. Yang and R.L. Mills in 1954 [55], turn out to be instrumental. Yang-Mills theories, contrary to the Abelian theory of Quantum Electrodynamics, are based on non-Abelian gauge symmetry, leading to a self-interaction of the massless gauge bosons. Like it was shown by t'Hooft and Veltman for the electroweak theory [56], if anomalies are cancelled [57, 58], which requires an appropriate representation of fermions, Yang-Mills theories were shown to be renormalizable by t'Hooft in 1971 [59]. Finally Nambu [34] as well as Fitch, Gell-Mann and Leutwyler [60] proposed to gauge the color symmetry and extend the Standard Model to  $SU_L(2) \times U_Y(1) \times SU_C(3)$  to also include the strong interacting sector. As it turns out  $SU_C(3)$  is also the only semi-simple compact Lie-group possible for the theory of strong interactions. A further step to establish QCD was taken by Gross and Wilczek [61] and Politzer [62], who proved by a 1-loop calculation that the coupling constant of QCD decreases with growing energies, contrary to the case of Abelian gauge groups. This property is called asymptotic freedom and allows to perform perturbative calculations in QCD at sufficiently high energies where the coupling constant is small. This is also compatible with the parton model since at high energies the partons effectively become non-interacting.

To build a bridge from the theoretical to the experimental side and to establish QCD as the right theory of the strong interaction the development of the operator product expansion by Wilson [63], cf. also [64–68], was essential. The operator product expansion allowed to systematically separate the physics at large distances from the physics at small distances and had direct applications to DIS in the form of the light-cone expansion, since the scattering can be described by the product of two electromagnetic current operators [69, 70]. Furthermore, it can be shown that the cross section is dominated by contributions at light-like distances. Therefore, an expansion around the light-cone, the so called light-cone expansion (LCE) [65, 71, 72], can be successfully applied. This expansion allows one to express the product of currents through the product of matrix elements of local operators, which describe the physics at long distances, and Wilson coefficients, which describe

the physics at short distances. Since QCD is asymptotically free, the Wilson coefficients can be calculated perturbatively at high energies. The matrix elements of local operators are regular in the limit of light-like separations, only the Wilson coefficients carry the singular structure in this limit. The relevance of the operators depend on their singular behavior which in turn is determined by a quantity called twist [73]. The twist can be calculated as the difference between the operator's canonical dimension and its spin. Operators with lowest twist are most relevant. For DIS the first contributing operators are of twist-2.

Since QCD is not a free theory, contrary to the assumptions of the naive parton model, there are interactions between the quarks inside the proton. In the consistent theoretical setup of the LCE, called the renormalization group improved parton model, it is possible to calculate the scaling of the structure functions from first principles. It turned out that the twist-2 approximation of the LCE reproduces Feynman's parton model in lowest order of perturbation theory [73], but it was also possible to go beyond this first approximation. It turned out that higher order corrections lead to logarithmic scaling violations in  $Q^2$  and that Bjorken scaling is therefore only approximately realized in QCD. The scale evolution is governed by the renormalization group equations and in particular the anomalous dimensions of the local operators emerging in the LCE. At leading order these were calculated in [74–86] and thus enabled quantitative predictions of the scaling violations in the limited kinematic regions probed in the early 1970s. Indeed, subsequent experimental efforts [87, 88] found agreement between the scaling violations predicted by QCD and experimental data. This prediction of logarithmic scaling violations has been, and still provides, one of the strongest experimental evidences for the theory of QCD and led to the broad acceptance of the theory in the early days of the Standard Model. Mathematically the LCE is naturally expressed in Mellin space. However, by an inverse Mellin transformation it is possible to express the renormalization group equations and anomalous dimensions in Bjorken's variable  $x$ , describing the momentum fraction of the parton [65, 89–94]. In the leading twist approximation the contributing quantities can be given an intuitive interpretation in the partonic picture [95–99]. The matrix elements of the local operators correspond to parton distribution functions which describe the probability to find a parton with a specific momentum fraction inside the proton. Their scale dependence is described by a set of integro-differential equations. The anomalous dimensions of the local operators are equivalent to the splitting functions  $P_{ij}$  which encode the probability to find a parton  $i$  when probing a parton  $j$  at different momentum fractions.

One of the last steps in the completion of the Standard Model was the discovery of heavy quarks, namely the charm ( $c$ ), bottom ( $b$ ) and top ( $t$ ) quark. The charm quark was discovered at the same time at SLAC and BNL in 1974. At SLAC two narrow resonances, named  $\Psi$  and  $\Psi'$ , were discovered at 3.1 GeV and 3.7 GeV in  $e^+e^-$  collisions respectively. At BNL another resonance, called  $J$ , was discovered in proton-proton collisions. These turned out to be the same particle, nowadays called  $J/\Psi$ . The existence of this resonance could not be explained by the three known quark flavors and was interpreted as a meson made up of a new quark, the charm quark. Its existence had been predicted on theoretical grounds before [100–105], since it is necessary to cancel anomalies in the second family [106, 107] and to suppress flavor changing neutral currents through the Glashow-Iliopoulos-Maiani mechanism [108] which could in principle be possible in the Standard Model but were not observed experimentally. The charm quark mass of  $m_c(m_c) = (1.28 \pm 0.03) \text{ GeV}$ , given in the  $\overline{\text{MS}}$ -scheme, makes it significantly heavier than the previously known light quarks,

$$m_u = 2.16_{-0.26}^{+0.49} \text{ MeV}, \quad m_d = 4.67_{-0.17}^{+0.48} \text{ MeV}, \quad m_s = 93_{-5}^{+11} \text{ MeV}$$

and even the proton and the neutron  $m_P \sim m_N \sim 940 \text{ MeV}$  [109]. In 1977 another resonance which could not be explained by the now known four quarks was found at FermiLab [110]. It was called  $\Upsilon$  and was interpreted as a bound state of a new type of quark and antiquark, the bottom quark with a mass of  $m_b(m_b) = 4.18_{-0.02}^{+0.03} \text{ GeV}$  [109], also given in the  $\overline{\text{MS}}$ -scheme. The

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fermionic content of the Standard Model was completed in 1995 when the top quark was discovered at the **Tevatron** at FermiLab [111–113]. Its pole mass of  $m_t = (173.1 \pm 0.9) \text{ GeV}$  [109] let it escape experimental discovery until facilities with much higher energies were available, although virtual effects were observed in  $B^0 - \bar{B}^0$  oscillations before [114]. Because of this exceptionally high mass the top quark decays too quickly to form bound state resonances.

The final experimental verification of the electroweak theory spanned an even longer time line, since not only the heavy gauge bosons, but also the mechanism of spontaneous symmetry breaking proposed by Higgs, Englert and Kibble [115–118], which effectively gives the electroweak gauge bosons their masses, needed to be experimentally verified. Where the charged gauge bosons  $W^\pm$  are easily seen in nuclear  $\beta$  decays, the neutral  $Z$  boson needed large collider based experiments and was finally discovered in the **Gargamelle** bubble chamber at CERN in 1973 [119]. The precise determination of its properties - like its mass and width - at the  $e^+e^-$  collider LEP and later LEP2 are now one of the most stringent tests of the electroweak theory and experimentally tests perturbative higher order corrections. Through virtual corrections it was also possible to derive estimates of the Higgs boson mass. The first experiment reaching the energy and luminosity to probe the range indicated by the indirect measurements was the Large Hadron Collider (LHC). In 2012, shortly after data taking, the Higgs boson was discovered at  $m_H \sim 125 \text{ GeV}$  [120, 121]. Therefore all particles predicted by the Standard Model are now experimentally discovered.

To probe the internal structure of the proton, many experiments to measure deep-inelastic scattering were built. Because of their experimental simplicity the first ones were fixed target experiments, where a high energetic electron beam was collided with a target which essentially provided the hadrons. Later, also collider experiments which allowed the exploration of larger values of the virtuality  $Q^2$  and smaller values of the Bjorken variable  $x$  were constructed. The experiment with the largest kinematic range so far has been the HERA collider at DESY in Hamburg [122, 123]. Three experiments, H1 [124], ZEUS [125] and HERMES [126], measured the structure functions in the kinematic range  $Q^2 = 0.045 \text{ GeV}^2$  to  $50\,000 \text{ GeV}^2$  and  $6 \times 10^{-7} \leq x \leq 0.65$  [123] or of parts thereof.

The more and more precise knowledge of the structure functions also required efforts on theoretical side. Higher order corrections beyond the leading order (LO) in QCD were needed. The one-loop corrections to the massless Wilson coefficients relevant for unpolarized DIS were calculated in [74, 127, 128] in the late 1970s. Additionally, the next-to-leading order (NLO) corrections to the anomalous dimensions were obtained [75–86]. The two-loop QCD corrections to the massless Wilson coefficients were completed during the following 15 years [86, 129–138]. The progression to next-to-next-to-leading order (NNLO) was first pursued for sum rules [139] and some fixed moments of the anomalous dimensions and Wilson coefficients [140–144]. The analytic results for general values of the Mellin variable  $N$  and momentum fraction  $x$  were obtained in [145, 146]. At four-loop order the analytic structure of the non-singlet anomalous dimension has been inferred from a series of moments [147] and a few moments for the five-loop non-singlet anomalous dimension have been calculated [148]. Like many massless single-scale quantities the analytic expressions of the anomalous dimensions and massless Wilson coefficients can be represented in terms of nested harmonic sums [149, 150] in  $N$  space and iterated integrals over a very restricted set of letters, the harmonic polylogarithms (HPLs) [151], in  $x$  space.

In addition to the case of unpolarized scattering, where one sums over all polarizations of the nucleon and lepton spin, the scattering of polarized leptons and hadrons has also been considered experimentally and theoretically. This setup is of special interest since polarized scattering can give insight into the spin structure of the nucleons. In the case of polarized scattering, new operators and additional independent structure functions appear. The theoretical predictions therefore need the separate calculation of polarized anomalous dimensions and Wilson coefficients. In the polarized case the anomalous dimensions have been calculated up to NNLO in the so called  $M$ -scheme [152]. The LO results were derived in [96, 153, 154], the NLO ones in [155–157] and the NNLO in [158, 159]. The Wilson coefficients for the structure function  $g_1$  are only known up to  $\mathcal{O}(\alpha_s^2)$  [160, 161].

Another structure function  $g_2$  is related to  $g_1$  by the Wandzura-Wilczek relation [162] at the level of twist-2.

The factorization of the perturbative and non-perturbative contribution using the LCE requires the partonic states to be strictly massless. For the light up, down and strange quarks this approximation is generally justified. However, the heavy quarks cannot be treated as massless over the whole kinematic range. The top quark is too heavy, so it has not been produced in the DIS experiments so far, the effects of the charm and bottom mass need to be considered, however. Theoretical calculations for massive quarks have been carried out soon after the discovery of the charm quark. The leading order contributions were calculated in [163–167]. It turned out that the scaling behavior of the heavy quarks differs from the one of massless quarks and that at low values of  $x$  the heavy quarks can lead to sizeable contributions. The heavy quark contributions therefore give a handle on the otherwise loosely determined gluon distribution at small  $x$ . The NLO corrections have been carried out for unpolarized scattering in [168–170] and for polarized scattering in [171–177].

The NLO corrections to massive DIS have been calculated semi-analytically in [168–170, 177], i.e. the integration over the last two invariants of the phase space have to be done numerically. Only the non-singlet contribution is known analytically [173, 178]. This is due to the fact that the integration over the massive phase space leads to analytic structures not covered by harmonic polylogarithms and needs the integration over kinematic square-roots and is therefore not easily achieved. However, it was discovered that the Wilson coefficients again factorize in the asymptotic region, i.e.  $Q^2 \gg m^2$  [179]. In the region where power correction  $m^2/Q^2$  can be ignored the massive Wilson coefficients factorize in Mellin space into the simple product of the massless Wilson coefficients and massive operator matrix elements (OMEs). The OMEs are matrix elements of the light cone operators between partonic states. They carry all the remaining mass dependence in the asymptotic limit and are process independent. All the process dependence is encoded in the massless Wilson coefficients. It was found, by comparing the asymptotic results with the semi-analytic results for the full mass dependence [180], that for the structure function  $F_2(x, Q^2)$  the asymptotic result holds for  $Q^2 \gtrsim 10m^2$ , a region where also higher twist contributions can be safely neglected [181], at the percent level. This covers a large part of the kinematics relevant for HERA. However, for the structure function  $F_L(x, Q^2)$  the asymptotic region is only reached for  $Q^2 \gtrsim 800m^2$ . More precise estimates will be given for the pure-singlet Wilson coefficients in the unpolarized and polarized case based on a fully analytic calculation of the full mass dependence in this thesis.

The OMEs are not only useful to calculate Wilson coefficients but also allow to define PDFs in the variable flavor number scheme (VFNS) [176, 180, 182]. The VFNS allows to treat the heavy quarks as effectively massless at high enough scales  $Q^2 \gg m^2$ . More precisely it matches PDFs obtained in a scheme with  $N_F$  massless flavors to a scheme where one or two additional quarks can be treated effectively massless, i.e. a  $N_F + 1$  or  $N_F + 2$  massless flavor scheme, at some high energy scale  $\mu$ . At high scales the heavy flavors also obtain a PDF, which is generated perturbatively. The matching coefficients between the PDFs at  $N_F$  and  $N_F + i$ ,  $i = 1, 2$ , massless flavors are given by the OMEs. The full VFNS can be determined by requiring an observable, like the structure functions, to be smooth while going from one to the other scheme. The VFNS is important to define PDFs at high virtualities needed at the LHC, cf. [183]. Here processes can also be initiated by the heavy quarks in the initial state.

The polarized NLO massive OMEs necessary for the evaluation of the structure functions have been calculated in [173]. The unpolarized case has been considered in [179, 180]. They were checked by an independent recalculation in [184, 185] and also the linear terms in the dimensional regulator were obtained later [186, 187]. These terms are needed for the renormalization of the massive OMEs at NNLO. The recalculation was not only valuable as a cross check, the techniques of directly integrating the Feynman parameter integrals in  $N$  space by means of Mellin-Barnes representations [188–191] and higher hypergeometric function techniques [192–195] rather than using a pool of precomputed integral identities opened up the opportunity to tackle the NNLO computation. Since the NNLO order

## 1. Introduction

contributions to the anomalous dimensions and massless Wilson coefficients are already known, the computation of the NNLO OMEs allows the calculation of the heavy quark effects in the asymptotic region at NNLO. The first step to this calculation was taken in 2009 by extending the formalism of renormalization to 3-loop order<sup>1</sup> and calculating a series of moments for the massive OMEs [176, 182, 196], needed to cross-check the all  $N$  solutions. At fixed values of the Mellin variable  $N$  it was possible to map the diagrams to massive tadpoles which can be evaluated using the program MATAD [197] written in FORM [198, 199]. Later the formalism was extended to handle two heavy quarks, the charm and the bottom quark, at the same time. Here the OMEs for a single heavy quark are crucial ingredients. In the limit  $\eta \ll 1$  moments of the operator matrix elements can be calculated in an expansion in  $\eta$  with Q2E/EXP [200, 201] which does a naive expansion in the mass ratio and uses MATAD to evaluate the single mass tadpoles. The first three moments up to  $\mathcal{O}(\eta^3)$  have been calculated in [202] together with the analytic results for general values of  $N$  and  $x$  for OMEs where the  $N$  dependence factorizes. To make phenomenological predictions the result for general values of  $N$  needs to be known. This calculations require more elaborate techniques than the calculation of fixed moments. The techniques developed will be presented throughout this thesis, since they are also crucial in obtaining the results presented here.

The process of DIS was important to establish QCD as the correct theory of the strong interaction. Nowadays the precise experimental data allow to determine the non-perturbative PDFs from the structure functions and to determine the fundamental parameters of the theory, most importantly the strong coupling constant  $\alpha_s$ , which can be extracted from data with an accuracy of  $\mathcal{O}(1\%)$  in NNLO analyses [203–207]. Since all of these quantities are universal, i.e. they are not process dependent, they provide a crucial input for the experiments at the LHC. Although running at a much higher center of mass energy  $\sqrt{s} = 13\text{TeV}$  than HERA, the knowledge of the anomalous dimensions and heavy mass OMEs at NNLO allows a precise evolution of these quantities and the description of the VFNS at NNLO. Furthermore, the NNLO heavy flavor contributions to DIS will allow to also push the determination of the heavy quark masses  $m_c$  and  $m_b$  in DIS from NLO and approximate NNLO [208] to a full NNLO analysis. This thesis is dedicated to further contribute to the understanding of heavy flavor production in DIS.

The thesis has the following structure. In Chapter 2 a theoretical overview of the deep-inelastic scattering process is given. First a description of the kinematics, the appearing structure functions and the factorization into parton distribution functions and Wilson coefficients and an understanding in the context of the parton model is given. Afterwards we will focus on the massive Wilson coefficients. Their factorization in the asymptotic limit  $Q^2 \gg m^2$  into the massless Wilson coefficient and the operator matrix elements will be shown and how to compute these quantities in a diagrammatic way. In the end, the variable flavor number scheme is introduced in detail.

In Chapter 3 the calculation of the massive pure singlet Wilson coefficients in the unpolarized case to  $\mathcal{O}(\alpha_s^2)$  is presented. After a general introduction, our method of direct integration in differential fields is presented, the full result is given by generalized iterated integrals over square root valued letters. In the following we give the expressions in the threshold and asymptotic region. We explicitly show that the asymptotic expression known from the massive operator matrix elements is reproduced. We also add power suppressed terms up to  $\mathcal{O}(m^4/Q^4)$  and evaluate the kinematic reach of these approximations. More terms in the expansion can be added in a straight forward way. Since the expansion only contains HPLs it is possible to use the expansions as a fast numerical implementation up to a certain kinematic point. In Chapter 4 we extend the discussion to the polarized pure-singlet Wilson coefficient. Since we have to work in dimensional regularization, we have to clarify our treatment of  $\gamma_5$  and introduce the Larin scheme and the finite renormalization associated with it [152, 209]. For other treatments of  $\gamma_5$  in dimensional regularization see for example Refs. [210–212].

In the next chapters we change topic and address the OMEs with two massive quarks. In Chapter 5

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<sup>1</sup>It was found that the renormalization at 2-loop was not entirely correct and needed modifications.

we recalculate the renormalization of the two mass OMEs, clarifying the notation in the previous treatment in [202]. During the recalculation of the renormalization it was also realized that the VFNS at NLO receives new contributions when decoupling the heavy charm and bottom quarks simultaneously instead of one after another. Since the charm and bottom masses do not form a large hierarchy, the ratio is given by

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

this procedure is preferable. These contributions to the VFNS at NLO are presented in the unpolarized case in detail in Chapter 6 together with a study of their numerical implications.

Chapter 7 is dedicated to the calculation of the missing NNLO two-mass OMEs in the unpolarized case. In Section 7.1 the two mass contributions to the pure-singlet operator matrix element is calculated. The calculation is based on Feynman parametrization and Mellin-Barnes integrals which will be introduced in more detail. Here it turns out that a closed form solution for general values of  $N$  is not easily possible since the associated difference equations do not factorize at first order. However, it is possible to find the momentum space solution by leaving one of the Feynman parameters unintegrated. In the analytic solution new structures with restricted support in the momentum fraction appear. The topic of Section 7.2 is the calculation of the two-mass contributions to the gluonic OME  $A_{gg,Q}^{(3)}$ . In this case all diagrams can be represented through one-dimensional Mellin-Barnes integrals and the residue sums factor to first order. The  $N$ -space solution contains up to generalized binomial sums which not only depend on the Mellin variable  $N$  but also on the mass ratio  $\eta$ . In momentum space these quantities can be represented via generalized iterated integrals whose letters contain square roots and also depend on the mass ratio  $\eta$ . Section 7.3 deals with the two-mass contributions to the OME  $\tilde{A}_{Qg}^{(3)}$ . Since the single mass OME  $A_{Qg}^{(3)}$  already contains elliptic sectors in the  $C_{A,F} T_F^2$  color factor a fully analytic treatment of the two-mass contributions seems out of reach at the moment. However, we introduce our algorithmic way to compute moments for the two-mass contributions in an expansion in the mass ratio  $\eta$ . Since the calculation is based on the differential and difference equations obeyed by master integrals and their generating function representation, the reduction to master integrals is introduced briefly. Moreover, an algorithm to calculate fixed moments of the master integrals is presented which could turn out to be useful in other two-scale problems as well.

In Chapter 8 the calculation of massive OMEs in the polarized case is discussed. First a new projector is presented, which allows us to treat the polarized calculation with the same techniques used in the unpolarized calculation. Then we present missing OMEs at NLO in the single mass case, which are crucial ingredients also for the renormalization of the NNLO results. We also present first results at NNLO for single and two-mass OMEs. The calculations at NNLO are the first independent cross-check on parts of the NNLO order anomalous dimensions calculated in Ref. [158].

In Chapter 9 the problem of QED initial state radiation in the process  $e^+ e^- \rightarrow \gamma^*/Z^*$  is addressed. Although it seems somewhat removed from the topics studied before, in the asymptotic limit it can be calculated using the same technique of massive operator matrix elements used in the previous chapters in the case of QCD. The corrections of  $\mathcal{O}(\alpha^2)$  were first calculated in [213] using direct integration and expansions under the integrals and were recalculated using the method of massive OMEs in [214]. The results, however, do not agree. This chapter therefore aims to clarify this matter. To be complete, we first present the corrections to  $\mathcal{O}(\alpha)$  in the full mass dependence and in the asymptotic expansion. Afterwards the  $\mathcal{O}(\alpha^2)$  corrections are presented. The corrections due to fermion pair production are complete and show agreement with the calculation of [214] but do deviate significantly from [213]. In Section 9.3.2 the contributions of soft photon radiation will be presented. They agree with Ref. [213]. The hard photonic corrections are work in progress and will not be addressed here. The last chapter contains the conclusions and an outlook for further studies. The Feynman diagrams in this thesis have been drawn using `Axodraw` [215] and `Axodraw 2` [216].





## 2. Deep Inelastic Scattering

### 2.1. The process of deep inelastic scattering

The most direct way to probe the structure of nucleons is deep-inelastic scattering. Here elementary particles not interacting strongly are colliding with a fixed target or a nucleon beam. Classically electrons, muons and neutrinos are used on the leptonic side and protons or neutrons as targets, for reviews about deep-inelastic scattering see for example Refs [217–219].

The Born process for the exchange of one gauge boson is depicted in Figure 2.1. A lepton with momentum  $k$  collides with a nucleon of momentum  $P$ . The lepton is scattered with momentum  $k'$ , while the nucleon disintegrates into a new hadronic state. In an inclusive manner we denote the outgoing momentum by  $P'$ .

We can choose different Lorentz invariant variables to describe the process. An important set are the virtuality of the gauge boson  $Q^2$ , the center-of-mass-energy  $s$  and the invariant mass of the hadronic final state,  $W$ , which are defined as

$$Q^2 = -q^2 = -(k - k')^2, \quad (2.1)$$

$$s = (k + P)^2, \quad (2.2)$$

$$W = (P + q)^2 = P'^2. \quad (2.3)$$

The virtuality  $Q^2$  measures the off-shellness of the exchanged gauge boson. In Born approximation it is equivalent to the Mandelstam variable  $t = -Q^2$ .

To describe the process one usually refers to the Bjorken variable  $x$ , the inelasticity  $y$  and the total energy transfer from the lepton to the nucleon in the nucleon's rest frame  $\nu$  [220]. They are defined via

$$\nu = \frac{P \cdot q}{M} = \frac{W^2 + Q^2 - M^2}{2M}, \quad (2.4)$$

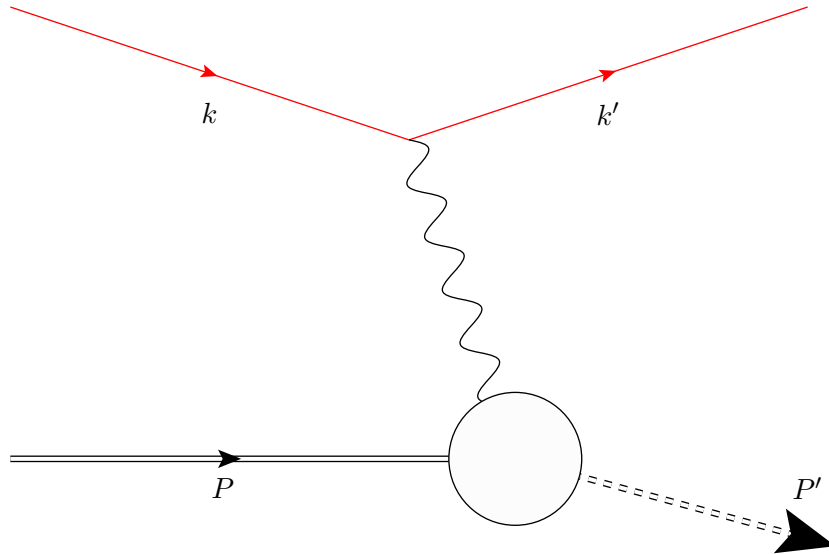


Figure 2.1.: Schematic picture of deep-inelastic electron proton scattering via single photon exchange.

## 2. Deep Inelastic Scattering

$$y = \frac{-q^2}{2P \cdot q} = \frac{Q^2}{2M\nu} = \frac{Q^2}{W^2 + Q^2 - M^2}, \quad (2.5)$$

$$x = \frac{P \cdot q}{P \cdot k} = \frac{2M\nu}{s - M^2 - m_l^2} = \frac{W^2 + Q^2 - M^2}{s - M^2 - m_l^2}, \quad (2.6)$$

with  $m_l$  the lepton and  $M$  the nucleon mass. In the target system, the inelasticity reflects how much energy has been transferred from the leptonic to the hadronic system relative to the energy of the incoming lepton,  $y = (E_{\text{TS}} - E'_{\text{TS}})/E_{\text{TS}}$ .

In the following we will consider neutral current reactions and deal with virtual photon exchange only. This is a valid picture for not too high virtualities  $Q^2 < 500 \text{ GeV}^2$ . We assume the QED and electroweak virtual corrections to have been carried out [221–223].

One speaks of deep-inelastic scattering if the virtuality  $Q^2$  and the invariant mass of the final state  $W^2$  are sufficiently large. A reasonable requirement for neutron and proton targets is  $Q^2 \geq 4 \text{ GeV}^2$  and  $W^2 \geq 4 \text{ GeV}^2$  [224]. For these values the continuum contributions dominate over the hadronic resonances and information about the nucleon substructure can be extracted. In the following discussions we will neglect the lepton mass  $m_l$  and drop terms of order  $M^2/Q^2$ . These target mass corrections can become important for low values of  $Q^2$  and larger values of  $x$  [225–231].

The leptons and nucleons are both fermions of spin 1/2. We describe the nucleon spin by the four-vector  $S$ , normalized in such a way that  $S^2 = -M^2$ . The vector can be split into a longitudinal and transverse component, since it has to fulfill  $P \cdot S = 0$ . If we align the  $z$ -axis with the beam direction, the spin vector takes the particular simple form

$$S_L = M(0, 0, 0, 1), \quad S_T = M(0, \cos(\beta), \sin(\beta), 0), \quad (2.7)$$

where  $\beta$  parametrizes the angle spanned by the nucleon spin in the plane transverse to the beam axis.

The physical region of DIS is constrained by several conditions. Since the proton is the lightest baryon and baryon number is conserved, we have

$$W^2 > M^2, \quad (2.8)$$

and

$$\nu \geq 0, \quad 0 \leq y \leq 1, \quad s \geq M^2. \quad (2.9)$$

From (2.8) and

$$W^2 = (P + q)^2 = M^2 + \frac{1-x}{x}Q^2 \quad (2.10)$$

we can conclude the physical region of the Bjorken variable

$$0 \leq x \leq 1. \quad (2.11)$$

We can see that  $x = 1$  describes the quasi-elastic process whereas  $x < 1$  describes the inelastic region.

The kinematics is additionally constrained by the parameters of the experiment under consideration. For example the HERA experiment [232] collided a proton beam at 820 GeV and 920 GeV and a lepton beam at 27.5 GeV. This resulted in a center-of-mass energy of  $\sqrt{s} = 300 \text{ GeV}$  and 319 GeV. Additionally the  $x$  region which is probed is constrained by

$$x = \frac{Q^2}{y(s - M^2)} \approx \frac{Q^2}{s} = \frac{Q^2}{10^5 \text{ GeV}^2}. \quad (2.12)$$

## 2.2. Cross section and structure functions

For the calculation of cross sections in deep inelastic electron-proton scattering, we consider the tree-level transition matrix element for the one photon exchange [69]

$$\mathcal{M} = \bar{u}(k', \lambda') \gamma_\mu u(k, \lambda) \frac{e^2}{q^2} \langle P', S' | J_\gamma^\mu(0) | P, S \rangle, \quad (2.13)$$

where  $u$  and  $\bar{u}$  are Dirac spinors which describe the initial and final state leptons with helicities  $\lambda$  and  $\lambda'$  respectively. The nucleon in the initial state with the momentum  $P$  and spin  $S$  is characterized by the state vector  $|P, S\rangle$  while the final state hadron is described by  $|P', S'\rangle$ .

The particular form of (2.13) allows to factor the cross section into a contribution from the leptons, forming the leptonic tensor  $L_{\mu\nu}$ , and the one from the hadrons, forming the hadronic tensor  $W_{\mu\nu}$ . The leptonic tensor can be easily calculated within the framework of perturbative QED, while the hadronic tensor contains non-perturbative hadronic contributions from long-distance QCD effects. To calculate these effects from first principles, non-perturbative approaches like QCD lattice simulations have to be performed. For the differential cross section we obtain [69]

$$\frac{d^2\sigma}{dx dy} = \frac{\alpha^2}{Q^4} L_{\mu\nu} W^{\mu\nu}, \quad (2.14)$$

with the fine structure constant  $\alpha = e^2/4\pi$ . The leptonic tensor reads

$$\begin{aligned} L_{\mu\nu} &= \sum_{\lambda, \lambda'} [\bar{u}(k', \lambda') \gamma_\mu u(k, \lambda)]^{\text{h.c.}} [\bar{u}(k', \lambda') \gamma_\nu u(k, \lambda)] \\ &= \text{Tr} [k \gamma_\mu k' \gamma_\nu] \\ &= 4 \left( k_\mu k'_\nu + k'_\mu k_\nu - \frac{Q^2}{2} g_{\mu\nu} \right). \end{aligned} \quad (2.15)$$

To obtain the differential cross section for inclusive scattering we have to insert the squared matrix element  $|\mathcal{M}|^2$  into the cross section and sum over all allowed final states. For unpolarized scattering we have to average over the initial state spins.

Although the hadronic tensor cannot be calculated explicitly, it can be described by different Lorentz structures and their respective structure functions by using Lorentz invariance and general symmetry considerations. In general 14 independent structure functions appear [228, 233]. For single photon exchange not only Lorentz but also time-reversal symmetry is obeyed. Using these symmetries only four possible tensor structures remain. The hadronic tensor can thus be expressed as

$$\begin{aligned} W_{\mu\nu} &= \frac{1}{4\pi} \sum_{S, P'} (2\pi)^4 \delta(P' - q - P) \langle P, S | J_\mu(0) | P' \rangle \langle P' | J_\nu(0) | P, S \rangle \\ &= \frac{1}{2x} \left( -g_{\mu\nu} + \frac{q_\mu q_\nu}{Q^2} \right) F_1(x, Q^2) \\ &+ \frac{2x}{Q^2} \left( P_\mu P_\nu + \frac{q_\mu P_\nu + q_\nu P_\mu}{2x} - \frac{Q^2}{4x^2} g_{\mu\nu} \right) F_2(x, Q^2) \\ &+ i\varepsilon_{\mu\nu\rho\sigma} \left( \frac{q^\rho S^\sigma}{P \cdot q} g_1(x, Q^2) + \frac{q^\rho [(P \cdot q) S^\sigma + (S \cdot q) p^\sigma]}{(P \cdot q)^2} g_2(x, Q^2) \right). \end{aligned} \quad (2.16)$$

$$(2.17)$$

Instead of  $F_1$  the structure function

$$F_L(x, Q^2) = F_2(x, Q^2) - 2xF_1(x, Q^2) \quad (2.18)$$

## 2. Deep Inelastic Scattering

is sometimes used in the literature. Inserting the leptonic and hadronic tensors into the formula (2.14) yields the differential cross section. For unpolarized DIS and single photon exchange we obtain [224]

$$\frac{d^2\sigma^{\gamma,\text{unpol}}}{dxdy} = \frac{2\pi\alpha^2}{xyQ^2} \{ [1 + (1-y)^2] F_2(x, Q^2) - y^2 F_L(x, Q^2) \}, \quad (2.19)$$

while for polarized DIS the cross section is given by [224]

$$\frac{d^2\sigma^{\gamma,\text{pol}}}{dxdy} = \frac{2\pi\alpha^2}{Q^4} \lambda_N^p f^p s [S_1^p(x, y) g_1(x, Q^2) + S_2^p(x, y) g_2(x, Q^2)]. \quad (2.20)$$

Here we use  $p$  to distinguish between longitudinal ( $p = L$ ) and transversal ( $p = T$ ) polarization. The degree of polarization of the nucleon is denoted by  $\lambda_N^p$  and the other terms are given by

$$\begin{aligned} f^L &= 1, & f^T &= \cos(\beta - \phi) \frac{d\phi}{2\pi} \sqrt{\frac{4M^2x}{sy} \left[ 1 - y - \frac{M^2xy}{s} \right]} \\ S_1^L(x, y) &= 2xy \left[ (2-y) - 2\frac{M^2}{s}xy \right], & S_1^T(x, y) &= 2xy^2 \\ S_2^L(x, y) &= -8x^2y \frac{M^2}{s}, & S_2^T(x, y) &= 4xy. \end{aligned} \quad (2.21)$$

The angle  $\phi$  is the azimuthal angle of the outgoing lepton. In the case of transverse nucleon polarization there is a non-trivial dependence on this angle remaining. In this case  $\beta$  is the direction of the nucleon spin in the transverse plane, see (2.7).

The structure functions  $F_2$  and  $F_L$  can be obtained from the hadronic tensor by applying the following projection operators

$$F_2 = \frac{2x}{d-2} \left[ (d-1) \frac{4x^2}{Q^2} P^\mu P^\nu W_{\mu\nu}(q, P) - g^{\mu\nu} W_{\mu\nu}(q, P) \right], \quad (2.22)$$

$$F_L = \frac{8x^3}{Q^2} P^\mu P^\nu W_{\mu\nu}(q, P). \quad (2.23)$$

The structure functions  $g_1$  and  $g_2$  need a more special treatment, since the Levi-Civita tensor

$$\varepsilon_{\mu\nu\rho\sigma} = \begin{cases} +1, & \text{for even permutations} \\ -1, & \text{for odd permutations} \\ 0, & \text{otherwise} \end{cases} \quad (2.24)$$

and  $\varepsilon_{0123} = +1$  cannot be defined in general space-time dimensions, which is needed for dimensional regularization. We will postpone this issue to Chapter 4.

## 2.3. The parton model

Bjorken investigated the hadronic tensor by using current algebra, assuming commutation rules for the currents corresponding to the ones for free fields. He predicted that in the Bjorken limit, i.e.  $Q^2 \rightarrow \infty$  and  $\nu \rightarrow \infty$  while  $Q^2/\nu = \text{const}$ , the structure functions become independent of  $Q^2$  [43]. This behavior leads to the natural variable  $x$ , c.f. (2.6), to describe the Bjorken limit and became later known as scaling. This scaling behavior was confirmed shortly after Bjorken's prediction by experiments at SLAC [38, 39, 234].

The observation that the cross section remains high at large momentum transfer  $Q^2$  shows similarities to the classical experiment by Rutherford [14] in which he collided  $\alpha$ -particles with a gold foil and favours scattering from point like particles. However, the size of the proton was known to be non negligible with a smooth charge distribution [21, 24, 235]. With the parton model Feynman was able to resolve these seemingly contradicting observations [44–46]. In his model the proton consists out of several point-like constituents, called partons. Therefore the lepton scatters off these partons by exchange of a photon. This highly virtual photon is assumed to scatter at a much smaller time scale as the self-interaction of the partons take place. This way the photon only sees the partons with *frozen* internal interactions and thus scatters from a single parton. Assuming collinear partons we can write the momentum of the incoming parton  $p$  as  $p = \xi P$ , where  $P$  is the momentum of the incoming proton. Therefore  $\xi$  can be referred to as momentum fraction. The momentum of the final state parton is denoted by  $p'$ . Then the squared matrix element of the partonic subprocess reads similarly to the leptonic tensor

$$|\mathcal{M}_q|^2 = 2e_q^2(p_\mu p'_\nu + p_\nu p'_\mu - p \cdot p' g_{\mu\nu}). \quad (2.25)$$

Here  $e_q$  denotes the electromagnetic charge of the parton  $q$ . The hadronic tensor is consequently given by the incoherent sum of the partonic subprocesses weighted with the probability to find the respective parton at a specific momentum fraction  $f_q(\xi)$ . The equation reads

$$\mathcal{W}_{\mu\nu} = \frac{1}{4\pi} \sum_q \int_0^1 d\xi f_q(\xi) |\mathcal{M}_q|^2 2\pi\delta(p'^2), \quad (2.26)$$

where the sum is over all parton species  $q$  found in the proton.

Inserting this hadronic tensor and the leptonic tensor from (2.15) into the formula for the differential cross section (2.14) leads to

$$\frac{d^2\sigma}{dxdy} = \frac{2\pi\alpha^2}{xyQ^2} \sum_q e_q^2 f_q(x) [1 + (1-y)^2]. \quad (2.27)$$

Comparing with the general formula in (2.19) we can extract the structure functions  $F_2$  and  $F_L$  as

$$F_2(x, Q^2) = x \sum_q e_q^2 f_q(x), \quad (2.28)$$

$$F_L(x, Q^2) = 0. \quad (2.29)$$

We see explicitly the scaling behavior of the structure functions in the parton model. Furthermore the vanishing of the structure function  $F_L(x, Q^2)$  implies the Callan-Gross relation [47]

$$F_2(x, Q^2) = 2xF_1(x, Q^2) \quad (2.30)$$

valid for spin- $\frac{1}{2}$  partons.

### 2.3.1. The light cone expansion for DIS

The hadronic tensor in Eq. (2.16) can also be rewritten via the absorptive part of the forward Compton amplitude  $T_{\mu\nu}$  using the optical theorem

$$W_{\mu\nu} = \frac{1}{\pi} \text{Im}(T_{\mu\nu}). \quad (2.31)$$

The forward Compton amplitude is given by

$$T_{\mu\nu} = i \sum_S \int d^4\xi e^{iq\xi} \langle P, S | T J_\mu(\xi) J_\nu(0) | P, S \rangle \quad (2.32)$$

$$= \frac{1}{2x} \left( g_{\mu\nu} + \frac{q_\mu q_\nu}{Q^2} \right) T_1(x, Q^2) + \frac{2x}{Q^2} \left( P_\mu P_\nu + \frac{P_\mu q_\nu + P_\nu q_\mu}{2x} - \frac{Q^2}{4x^2} g_{\mu\nu} \right) T_2(x, Q^2). \quad (2.33)$$

Here T denotes the time ordering operator. Again, Eq. (2.33) assumes the exchange of a single photon. Furthermore we restrict the discussion to unpolarized nucleons, the extension to the polarized case is straight forward.

To continue with the calculation we have to separate physics at perturbative and non-perturbative scales. For deep inelastic scattering the operator product expansion, pioneered by Wilson and others [63, 64, 66–68] turned out to be a useful tool. The operator product expansion was originally formulated to express a product of local operators in the limit of short distances as a product of regular operators and Wilson coefficients which carry the singular behavior in this limit. However, the product of current operators in the hadronic tensor of Eq. (2.32) needs to be treated differently. It can be shown that in the Bjorken limit contributions near the light cone

$$\xi^2 \leq \frac{1}{Q^2} \approx 0 \quad (2.34)$$

dominate. The generalization of the operator product expansion to light-like separations is also called light-cone expansion [65, 71, 72]. In this limit the time ordered product of currents can be represented by [63, 65, 71, 72]

$$\lim_{\xi^2 \rightarrow 0} T J(\xi) J(0) \sim \sum_{i, N, \tau} \bar{C}_{i, \tau}^N(\xi^2, \mu^2) \xi_{\mu_1} \dots \xi_{\mu_N} O_{i, \tau}^{\mu_1 \dots \mu_N}(0, \mu^2). \quad (2.35)$$

The  $O_{i, \tau}^{\mu_1 \dots \mu_N}(0, \mu^2)$  denote local operators and the  $\bar{C}_{i, \tau}^N(\xi^2, \mu^2)$  are their associated Wilson coefficients. Denoting the canonical dimensions of the local operator and the currents with  $D_O$  and  $D_J$  respectively and the global spin with  $N$ , they scale like

$$\bar{C}_{i, \tau}^N(\xi^2, \mu^2) \approx \left( \frac{1}{\xi^2} \right)^{\frac{N - D_O + D_J}{2}}. \quad (2.36)$$

Here a term which is often used is the twist of the local operator [73]

$$\tau = D_O - N, \quad (2.37)$$

which describes the scaling behavior induced by the local operator to the Wilson coefficient. Operators with the lowest twist dominate for large momentum transfer  $Q^2 \rightarrow \infty$ .

For the single photon exchange the operators of lowest twist  $\tau = 2$  are given by [236]

$$O_{q, r; \mu_1, \dots, \mu_N}^{\text{NS}} = i^{N-1} \mathbf{S}[\bar{\psi} \gamma_{\mu_1} D_{\mu_2} \dots D_{\mu_N} \frac{\lambda_r}{2} \psi] - \text{trace terms}, \quad (2.38)$$

$$O_{q; \mu_1, \dots, \mu_N}^{\text{S}} = i^{N-1} \mathbf{S}[\bar{\psi} \gamma_{\mu_1} D_{\mu_2} \dots D_{\mu_N} \psi] - \text{trace terms}, \quad (2.39)$$

$$O_{g;\mu_1,\dots,\mu_N}^S = 2i^{N-2} \mathbf{SSp}[G_{\mu_1\alpha}^a g^{\alpha\beta} D_{\mu_2} \dots D_{\mu_{N-1}} G_{\beta\mu_N}^a] - \text{trace terms} . \quad (2.40)$$

In the polarized case the operators

$$O_{q,r;\mu_1,\dots,\mu_N}^{\text{NS},5} = i^{N-1} \mathbf{S}[\bar{\psi}\gamma_5\gamma_{\mu_1} D_{\mu_2} \dots D_{\mu_N} \frac{\lambda_r}{2}\psi] - \text{trace terms} , \quad (2.41)$$

$$O_{q;\mu_1,\dots,\mu_N}^{\text{S},5} = i^{N-1} \mathbf{S}[\bar{\psi}\gamma_5\gamma_{\mu_1} D_{\mu_2} \dots D_{\mu_N}\psi] - \text{trace terms} , \quad (2.42)$$

$$O_{g;\mu_1,\dots,\mu_N}^{\text{S},5} = 2i^{N-2} \mathbf{SSp} \left[ \frac{1}{2} \varepsilon^{\mu_1\alpha\beta\gamma} G_{\beta\gamma}^a D_{\mu_2} \dots D_{\mu_{N-1}} G_{\alpha\mu_N}^a \right] - \text{trace terms} . \quad (2.43)$$

emerge. Here  $\mathbf{Sp}$  is the trace over the  $SU_C(3)$  algebra, and  $\mathbf{S}$  is the symmetrization operator

$$\mathbf{S}f_{\mu_1,\dots,\mu_M} = \frac{1}{M!} \sum_w f_w , \quad (2.44)$$

of the Lorentz indices  $\mu_1, \dots, \mu_N$  and  $w$  their permutations.  $D_\mu$  is the covariant derivative,  $\psi$  and  $\bar{\psi}$  are the quark and anti-quark fields, and  $G_{\mu\nu}^a$  the gluonic field strength tensor, with  $a$  the color index in the adjoint representation. Furthermore,  $\lambda_r$  is the flavor matrix of  $SU(N_F)$ . The labels  $q, g$  on the left-hand side of Eqs. (2.38-2.43) distinguish quarkonic and gluonic operators.

In the following, we will mainly work in Mellin space to take advantage of the simplicity of the emerging convolution formulae, which are given by ordinary products. The Mellin transform of a function  $f(x)$  is defined by [237]

$$M[f(x)](N) = \int_0^1 dx x^{N-1} f(x) . \quad (2.45)$$

or

$$M[[f(x)]_+](N) = \int_0^1 dx (x^{N-1} - 1) f(x) . \quad (2.46)$$

depending on the regularity of  $f(x)$  in the limit  $x \rightarrow 1$ . The inverse Mellin transformation is given by

$$f(x) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds x^{-s} M[f(x)](s) . \quad (2.47)$$

The contour of the integration runs parallel to the imaginary axis and  $c \in \mathcal{R}$  has to be chosen in such a way that the singularities of  $M[f(x)](s)$  lie to the left of the integration contour. The application of this formula requires the analytic continuation to complex arguments of the Mellin transform. From the knowledge of the Mellin moments of a function  $f(x)$  for either all even or all odd integers  $N$ , Carlson's theorem [238, 239] states that the analytic continuation is unique within a certain class of functions. For a more precise statement in the context discussed in this thesis see [240].

The convolution of two regular functions reads

$$[f \otimes g](z) = \int_0^1 dx_1 \int_0^1 dx_2 \delta(z - x_1 x_2) f(x_1) g(x_2) . \quad (2.48)$$

Its Mellin transform factors into the product of the Mellin transforms of both functions

$$M[f(z) \otimes g(z)](N) = M[f(z)](N) \cdot M[g(z)](N) . \quad (2.49)$$

## 2. Deep Inelastic Scattering

The convolution of a regular function with a function which needs regularization in the limit  $z \rightarrow 1$  reads [241]

$$M [[f(z)]_+ \otimes g(z)](N) = \int_0^1 dz z^{N-1} \left\{ \int_z^1 dy f\left(\frac{z}{y}\right) \left[ \frac{1}{y} g\left(\frac{x}{y}\right) - g(x) \right] - g(z) \int_0^z dy f(y) \right\}. \quad (2.50)$$

In what follows, we will use the Mellin transform to map between the momentum fraction  $z$ - and the Mellin  $N$ -spaces.

Inserting the operator product expansion for twist-2 one finds for the forward Compton amplitude for deep inelastic scattering [71, 72, 127, 217]

$$T_{\mu\nu} = \sum_{i,N} \left\{ [Q^2 g_{\mu\mu_1} g_{\nu\mu_2} + g_{\mu\mu_1} q_{\nu} q_{\mu_2} + g_{\nu\mu_2} q_{\mu} q_{\mu_1} - g_{\mu\nu} q_{\mu_1} q_{\mu_2}] C_{i,2}\left(N, \frac{Q^2}{\mu^2}\right) + [g_{\mu\nu} + \frac{q_{\mu} q_{\nu}}{Q^2}] q_{\mu_1} q_{\mu_2} C_{i,L}\left(N, \frac{Q^2}{\mu^2}\right) \right\} q_{\mu_3} \dots q_{\mu_N} \left(\frac{2}{Q^2}\right)^N \langle P | \mathcal{O}_i^{\mu_1 \dots \mu_N} | P \rangle. \quad (2.51)$$

Neglecting trace term we can rewrite the operator matrix elements as

$$\langle P | \mathcal{O}_i^{\mu_1 \dots \mu_N} | P \rangle = A_i \left(N, \frac{P^2}{\mu^2}\right) P^{\mu_1} \dots P^{\mu_N}, \quad (2.52)$$

which leads to the final expression for the forward Compton tensor

$$T_{\mu\nu}(q, P) = 2 \sum_{i,N} \left\{ \frac{2x}{Q^2} [P_{\mu} P_{\nu} + \frac{P_m u q_n u + P_{\nu} q_{\mu}}{2x} - \frac{Q^2}{4x^2} g_{\mu\nu}] C_{i,2}\left(N, \frac{Q^2}{\mu^2}\right) + \frac{1}{2x} [g_{\mu\nu} + \frac{q_{\mu} q_{\nu}}{Q^2}] C_{i,L}\left(N, \frac{Q^2}{\mu^2}\right) \right\} \frac{1}{x^{N-1}} A_i \left(N, \frac{P^2}{\mu^2}\right). \quad (2.53)$$

The sum is only convergent for  $x > 1$ , which is outside the physical region  $0 \leq x \leq 1$ . We can however continue the functions analytically.

Using the optical theorem we arrive at the expression for the Mellin moments for the structure functions

$$\begin{aligned} F_{(2,L)}(N, Q^2) &= M [F_{(2,L)}(x, Q^2)](N) \\ &= \sum_i C_{i,(2,L)} \left(N, \frac{Q^2}{\mu^2}\right) A_i \left(N, \frac{P^2}{\mu^2}\right), \end{aligned} \quad (2.54)$$

where the sum goes over the singlet, non-singlet and gluonic operators defined above. We see that the structure functions at twist-2 factorize into Wilson-coefficients and operator matrix elements.



### 2.3.2. Light flavor Wilson coefficients

Starting with parton distribution functions (PDFs) for each quark  $f_i(x)$  and the gluon  $G(x)$ , we can identify the non-perturbative vacuum expectation values of different operators with different combinations of these PDFs using their flavour symmetries. The gluon PDF can be identified with the gluon operator. The singlet operator can be identified with the singlet PDF defined by

$$\Sigma(x) = \sum_{k=1}^{N_f} [f_k(x) + f_{\bar{k}}(x)] \quad (2.55)$$

and the non-singlet operator with the non-singlet PDF

$$\Delta_k(x) = f_k(x) + f_{\bar{k}}(x) - \frac{\Sigma(x)}{N_f}. \quad (2.56)$$

$N_f$  is the number of massless flavors. This identification of the operator matrix elements with the parton distribution functions leads to the QCD-improved parton model. The structure functions are in turn given by

$$\begin{aligned} F_{(2,L)}(N_f, N-1, Q^2) &= \frac{1}{N_f} \sum_{k=1}^{N_f} e_k^2 \left[ \Sigma(N_f, N, \mu^2) C_{q,(2,L)}^S \left( N_f, N, \frac{Q^2}{\mu^2} \right) \right. \\ &\quad + G(N_f, N, \mu^2) C_{g,(2,L)}^S \left( N_f, N, \frac{Q^2}{\mu^2} \right) \\ &\quad \left. N_f \Sigma_k(N_f, N, \mu^2) C_{q,(2,L)}^{NS} \left( N_f, N, \frac{Q^2}{\mu^2} \right) \right]. \end{aligned} \quad (2.57)$$

It is convenient to decompose the singlet further into the pure singlet and the non-singlet contribution

$$C_{q,(2,L)}^S = C_{q,(2,L)}^{PS} + C_{q,(2,L)}^{NS}, \quad (2.58)$$

since single diagrams in the calculation only belong to either the non-singlet or the pure singlet contribution. Inserting this definition into (2.57), the non-singlet Wilson coefficient is multiplied by the PDF combination  $f_k(x) + f_{\bar{k}}(x)$  instead of  $\Sigma(x)$  and is therefore sometimes referred to as the non-singlet PDF combination in the earlier literature although not being a non-singlet object based on symmetries [179, 180].

The massless Wilson coefficients obey the following expansion in the strong coupling constant

$$C_{g,(2,L)}^S \left( n_f, N, \frac{Q^2}{\mu^2} \right) = \sum_{i=1}^{\infty} a_s^i C_{g,(2,L)}^{(i),S} \quad (2.59)$$

$$C_{q,(2,L)}^{PS} \left( n_f, N, \frac{Q^2}{\mu^2} \right) = \sum_{i=2}^{\infty} a_s^i C_{q,(2,L)}^{(i),PS} \quad (2.60)$$

$$C_{q,(2,L)}^{NS} \left( n_f, N, \frac{Q^2}{\mu^2} \right) = \delta_2 + \sum_{i=1}^{\infty} a_s^i C_{q,(2,L)}^{(i),NS} \quad (2.61)$$

with

$$\delta_2 = 1 \text{ for } F_2 \text{ and } \delta_2 = 0 \text{ for } F_L \quad (2.62)$$

and

$$a_s = \frac{\alpha_s}{4\pi} = \left( \frac{g_s}{4\pi} \right)^2. \quad (2.63)$$

## 2. Deep Inelastic Scattering

We have already introduced the factorization scale  $\mu$ , which artificially separates the high energetic, perturbative from the non-perturbative contributions. The total derivative with respect to  $\mu$  reads

$$\mathcal{D}(\mu^2) = \mu^2 \frac{\partial}{\partial \mu^2} + \beta(\mu^2) \frac{\partial}{\partial a_s(\mu^2)} - \gamma_m(\mu^2) m(\mu^2) \frac{\partial}{\partial m(\mu^2)} \quad (2.64)$$

Since physical quantities cannot depend on this arbitrary scale, the total derivative of these quantities with respect to  $\mu$  has to vanish. This gives rise to the renormalization group equations (RGEs), which can relate quantities at different energy scales with perturbatively calculable coefficient functions. The most notables are the  $\beta$ -function and the anomalous mass dimension  $\gamma_m$  which governs the running of the strong coupling constant and the masses respectively

$$\beta(\mu^2) = \mu^2 \frac{\partial a_s(\mu^2)}{\partial \mu^2}, \quad (2.65)$$

$$\gamma_m(\mu^2) = -\frac{\mu^2}{m(\mu^2)} \frac{\partial m(\mu^2)}{\partial \mu^2}. \quad (2.66)$$

For the renormalization of the operators, which will be dealt with in the next section, we also have to introduce multiplicative renormalization factors

$$\mathcal{O}_{q,r;\mu_1,\dots,\mu_N}^{NS} = Z^{NS}(\mu^2) \hat{\mathcal{O}}_{q,r;\mu_1,\dots,\mu_N}^{NS}, \quad (2.67)$$

$$\mathcal{O}_{i;\mu_1,\dots,\mu_N}^S = Z_{ij}^S(\mu^2) \hat{\mathcal{O}}_{i;\mu_1,\dots,\mu_N}^S, \quad (2.68)$$

in the massless case. These will absorb remaining collinear divergences into the PDFs.

The RGE of the structure function

$$\mathcal{D}(\mu^2) F_{(2,L)}(N, Q^2) = 0 \quad (2.69)$$

then leads to a particular  $\mu$ -dependence of the structure functions and PDFs given by

$$\frac{d}{d \ln \mu^2} \begin{pmatrix} C_{q,i}^S(N_f, N, \mu^2) \\ C_{g,i}(n_f, N, \mu^2) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \gamma_{qq} & \gamma_{gq} \\ \gamma_{gq} & \gamma_{gg} \end{pmatrix} \begin{pmatrix} C_{q,i}^S(n_f, N, \mu^2) \\ C_{g,i}(n_f, N, \mu^2) \end{pmatrix}, \quad (2.70)$$

$$\frac{d}{d \ln \mu^2} C_{q,i}^{NS}(n_f, N, \mu^2) = \frac{1}{2} \gamma_{qq}^{NS} C_{q,i}^{NS}(n_f, N, \mu^2), \quad (2.71)$$

$$\frac{d}{d \ln \mu^2} \begin{pmatrix} \Sigma(n_f, N, \mu^2) \\ G(n_f, N, \mu^2) \end{pmatrix} = -\frac{1}{2} \begin{pmatrix} \gamma_{qq} & \gamma_{gq} \\ \gamma_{gq} & \gamma_{gg} \end{pmatrix} \begin{pmatrix} \Sigma(n_f, N, \mu^2) \\ G(n_f, N, \mu^2) \end{pmatrix}, \quad (2.72)$$

$$\frac{d}{d \ln \mu^2} \Delta_k(n_f, N, \mu^2) = -\frac{1}{2} \gamma_{qq}^{NS} \Delta_k(n_f, N, \mu^2). \quad (2.73)$$

The  $\gamma_{ij}$  are also known as the Altarelli-Parisi splitting functions. They can be calculated order by order in perturbation theory. They are known up to NNLO [145, 146], the LO results can be found in [89, 90, 242], while the NLO results have been obtained in [74–80, 84, 243]. There are ongoing efforts to compute fixed moments for the N<sup>3</sup>LO splitting functions [147]. The parton densities are universal but non-perturbative and have to be extracted from experimental data. Their evolution provide a stringent test of QCD quantities.

### 2.3.3. Heavy flavor contributions

In the discussion above, we assumed all participating quarks to be massless. For the three light flavors this is justified, since their masses, cf. Chapter 1, are below the QCD-scale of  $\Lambda_{\text{QCD}} \approx 200 \text{ MeV}$ . This means that these flavors can be produced non-perturbatively in the proton, yielding the different parton distributions. The heavy quark flavors all have masses well above  $\Lambda_{\text{QCD}}$  [109]

$$m_c(m_c) = (1.28 \pm 0.03) \text{ GeV}, \quad m_b(m_b) = 4.18_{-0.03}^{+0.04} \text{ GeV}, \quad m_t = (173.1 \pm 0.6) \text{ GeV}. \quad (2.74)$$

This means that these flavors are only produced perturbatively, i.e. we cannot simply assign a parton distribution to these flavors. The masses of the charm and the bottom quark are given in the  $\overline{\text{MS}}$ -scheme, the top quark mass is the pole mass.<sup>1</sup> Since the energy of HERA was not large enough to produce top quarks, we will restrict ourself to the discussion of two heavy flavor. This is also justified, since the mass of the top quark is by far larger than the other mass scales. Therefore neglecting polynomial terms in the ratio  $m_c^2/m_t^2 = m_b^2/m_t^2 \approx 0$  is justified. However the simultaneous treatment of charm and bottom is necessary to keep track of polynomial terms in the squared mass ratio

$$\eta = \frac{m_c^2}{m_b^2} \approx 0.1. \quad (2.75)$$

Since these masses do not form a strong hierarchy these contributions can lead to sizable effects. Although Feynman diagrams with fermion lines of both heavy quarks appear from 3-loop order onwards, renormalization and scheme changes already have an effect at  $\mathcal{O}(a_s^2)$ . These effects will be explored in the context of the variable flavour number scheme in Chapter 6. Although the Wilson coefficients for one or two heavy flavors can in principle be calculated for the full mass dependence these calculations introduce multiple scales and grow in complexity quite rapidly with the number of loops. The non-singlet Wilson coefficient at NLO was calculated analytically in [173, 179] in the tagged flavor case and in the fully inclusive case in [178]. The calculation of the pure singlet Wilson coefficient at NLO will be addressed in Chapters 3 and 4. Here already elliptic structures emerge in the result. However in the asymptotic limit, i.e.  $Q^2 \gg m^2$ , the heavy flavor Wilson coefficients again factorize

$$C_{j,(2,L)} = \sum_i A_{ij} C_{i,(2,L)} + \mathcal{O}\left(\frac{m^2}{Q^2}\right). \quad (2.76)$$

Therefore, in the asymptotic limit, i.e. neglecting power corrections in the mass, the heavy flavor Wilson coefficients can be calculated using the massless Wilson coefficients and universal heavy flavor operator matrix elements

$$A_{ij} (p^{\mu_1} \dots p^{\mu_N} + \text{trace terms}) = \langle j | O_i^{\mu_1 \dots \mu_N} | j \rangle. \quad (2.77)$$

The external state  $j$  can be either a gluon  $g$  or a quark  $q$  and the index  $i$  labels the different operators. The operator matrix elements can be calculated through 2-point Green's functions with operator insertions. The Lorentz-structure factorizes from the OME and the external states are on-shell ( $p^2 = 0$ ). To simplify the calculation we contract with the source term

$$J_{\mu_1 \dots \mu_N} = \Delta_{\mu_1} \dots \Delta_{\mu_N}, \quad (2.78)$$

where  $\Delta$  is a arbitrary light-like vector ( $\Delta^2 = 0$ ). This way all trace terms vanish. Extracting all Dirac, Lorentz and color structures we can write

$$\bar{u}_k(p, s) \hat{G}_q^{\text{NS},kl} \lambda_r u_l(p, s) = J_{\mu_1 \dots \mu_N} \langle q, k | O_{q,r}^{\text{NS},\mu_1 \dots \mu_N} | q, l \rangle_Q, \quad (2.79)$$

<sup>1</sup>There is a discussion about the precise definition of the scheme in which the top quark mass is measured at the LHC. However, given the current errors the differences between the pole mass and the so called Monte-Carlo mass should be negligible, cf. [244].

## 2. Deep Inelastic Scattering

$$\bar{u}_k(p, s) \hat{G}_i^{kl} u_l(p, s) = J_{\mu_1 \dots \mu_N} \langle q, k | O_i^{\mu_1 \dots \mu_N} | q, l \rangle_Q, \quad i \in \{g, g, Q\} \quad (2.80)$$

$$\varepsilon^\mu(p) \hat{G}_{i, \mu\nu}^{ab} \varepsilon^\nu(p) = J_{\mu_1 \dots \mu_N} \langle g, \mu, a | O_i^{\mu_1 \dots \mu_N} | g, \nu, b \rangle_Q, \quad i \in \{g, g, Q\}. \quad (2.81)$$

The subscript  $Q$  denotes the presence of a heavy quark and  $k, l$  and  $a, b$  denote indices of the color group in the fundamental and adjoint representation, respectively. The operator introduces the Feynman rules summarized in Appendix B. In the unpolarized case they obey the following representation. To obtain the operator matrix elements from the corresponding Greens function, one has to apply the projector

$$P_q \hat{G}_{lq}^{ij} = \frac{\delta^{ij}}{N_c} (\Delta \cdot p)^{-N} \frac{1}{4} \text{tr} [\not{p} \hat{G}_l^{ij}] \quad (2.82)$$

in the quarkonic case. In the gluonic case we can choose the physical projector on transversal gluons

$$P_g^{(2), \mu\nu} \hat{G}_{l, \mu\nu}^{ab} = \frac{\delta_{ab}}{N_c^2 - 1} \frac{1}{D - 2} (\Delta \cdot p)^{-N} \left( -g^{\mu\nu} + \frac{p^\mu \Delta^\nu + p^\nu \Delta^\mu}{\Delta \cdot p} \right) \hat{G}_{l, \mu\nu}^{ab} \quad (2.83)$$

or the nonphysical one

$$P_g^{(1), \mu\nu} \hat{G}_{l, \mu\nu}^{ab} = -\frac{\delta_{ab}}{N_c^2 - 1} \frac{g^{\mu\nu}}{D - 2} (\Delta \cdot p)^{-N} \hat{G}_{l, \mu\nu}^{ab}. \quad (2.84)$$

In the latter case one also has to consider external ghosts which are projected using

$$P_{\text{ghost}} \hat{G}_{\text{ghost}}^{ab} = \frac{\delta_{ab}}{N_c^2 - 1} \frac{1}{D - 2} (\Delta \cdot p)^{-N} \hat{G}_{\text{ghost}}^{ab}. \quad (2.85)$$

Since the ghost diagrams have a much simpler structure than the terms induced by the physical projector one usually resorts to the second way of calculation. The number of colors is denoted by  $N_c$ , which for QCD equals  $N_c = 3$ . However, the results are calculated for the general  $SU(N)$  gauge group. The polarized case can be treated similarly but needs special attention because of the continuation of  $\gamma_5$  into arbitrary space-time dimensions. We will generally work in the Larin scheme [209] although other schemes exist [56, 210–212, 245–248]. In the Larin scheme one substitutes

$$\gamma_5 = \frac{i}{24} \gamma_\mu \gamma_\nu \gamma_\rho \gamma_\delta \varepsilon^{\mu\nu\rho\delta}. \quad (2.86)$$

For polarized quantities this will lead to the product of two Levi-Civita tensors. This product can be continued to  $d$ -dimensions using [249]

$$\varepsilon_{\alpha\beta\gamma\delta} \varepsilon_{\mu\nu\rho\delta} = \begin{vmatrix} g_{\alpha\mu} & g_{\alpha\nu} & g_{\alpha\rho} & g_{\alpha\sigma} \\ g_{\beta\mu} & g_{\beta\nu} & g_{\beta\rho} & g_{\beta\sigma} \\ g_{\gamma\mu} & g_{\gamma\nu} & g_{\gamma\rho} & g_{\gamma\sigma} \\ g_{\delta\mu} & g_{\delta\nu} & g_{\delta\rho} & g_{\delta\sigma} \end{vmatrix} \quad (2.87)$$

and interpreting the metrics in  $d$  dimensions. This scheme will in general, like all other known schemes for  $\gamma_5$ , break Ward-identities. Therefore, a final renormalization step in which these fundamental identities are restored, is necessary. This problem will be discussed further in Chapter 8.7 with special emphasis on the calculation of operator matrix elements for polarized scattering.

In the following we will give the contribution from heavy quarks to the inclusive structure functions in the fixed flavor number scheme (FFNS). This means that we work with a fixed number of massless and massive quarks, in contrast to a variable flavor number scheme (VFNS), where the number of massless and massive flavors changes depending on the energy scale under consideration. For HERA we have  $N_F = 3$  light flavors ( $u$ ,  $d$  and  $s$  quarks) and two heavy flavors ( $c$  and  $b$  quarks). In the

following the index  $N_F + 2$  has to be understood symbolically as  $N_F$  light and 2 heavy flavors. The relations for a single heavy quark flavor can be found in [182], while the two mass case was presented in [202]. For completeness we will summarize the results for the heavy flavor Wilson coefficients and the structure functions here. We distinguish heavy flavor Wilson coefficients where the photon couples to a light flavor  $L_i$  and those where it couples to a heavy quark flavor  $H_i$ . We will only present the expanded results up to  $\mathcal{O}(a_s^3)$ , to express these we introduce the expansions

$$A_{ij}(N_F) = \delta_{ij} + \sum_{k=1}^{\infty} a_s^k A_{ij}^{(k)}(N_F), \quad (2.88)$$

$$C_{ij}(N_F) = \delta_{ij} + \sum_{k=1}^{\infty} a_s^k C_{ij}^{(k)}(N_F), \quad (2.89)$$

for the OMEs and the massless Wilson coefficients. For brevity we will suppress the dependencies on  $N$  and the scales  $Q^2/\mu^2$  and  $m^2/\mu^2$ . In what follows we also use the notation

$$\tilde{f}(x) = \frac{f(x)}{x}, \quad (2.90)$$

$$\hat{f}(x) = f(x+2) - f(x). \quad (2.91)$$

With this notation and under the asymptotic condition

$$Q^2, \mu^2 \gg m_c^2, m_b^2, \quad (2.92)$$

we can write

$$\begin{aligned} L_{q,(2,L)}^{\text{NS}}(N_F + 2) &= a_s^2 \left[ A_{qq,Q}^{(2),\text{NS}}(N_F + 2) \delta_2 + \hat{C}_{q,(2,L)}^{(2),\text{NS}}(N_F) \right] \\ &+ a_s^3 \left[ A_{qq,Q}^{(3),\text{NS}}(N_F + 2) \delta_2 + A_{qq,Q}^{(2),\text{NS}}(N_F + 2) C_{q,(2,L)}^{(1),\text{NS}}(N_F + 2) \right. \\ &\quad \left. + \hat{C}_{q,(2,L)}^{(3),\text{NS}}(N_F) \right], \end{aligned} \quad (2.93)$$

$$\begin{aligned} L_{q,(2,L)}^{\text{PS}}(N_F + 2) &= a_s^3 \left[ A_{qq,Q}^{(3),\text{PS}}(N_F + 2) \delta_2 + A_{qq,Q}^{(2)}(N_F + 2) N_F \tilde{C}_{g,(2,L)}^{(1)}(N_F + 2) \right. \\ &\quad \left. + N_F \hat{\tilde{C}}_{q,(2,L)}^{(3),\text{PS}}(N_F) \right], \end{aligned} \quad (2.94)$$

$$\begin{aligned} L_{g,(2,L)}^{\text{S}}(N_F + 2) &= a_s^2 A_{gg,Q}^{(1)}(N_F + 2) N_F \tilde{C}_{g,(2,L)}^{(1)}(N_F + 2) \\ &+ a_s^3 \left[ A_{gg,Q}^{(3)}(N_F + 2) \delta_2 + A_{gg,Q}^{(1)}(N_F + 2) N_F \tilde{C}_{g,(2,L)}^{(2)}(N_F + 2) \right. \\ &\quad + A_{gg,Q}^{(2)}(N_F + 2) N_F \tilde{C}_{g,(2,L)}^{(1)}(N_F + 2) \\ &\quad \left. + A_{Qg}^{(1)}(N_F + 2) N_F \tilde{C}_{q,(2,L)}^{(2),\text{PS}}(N_F + 2) + N_F \hat{\tilde{C}}_{g,(2,L)}^{(3)}(N_F) \right], \end{aligned} \quad (2.95)$$

$$\begin{aligned} \tilde{H}_{q,(2,L)}^{\text{PS}}(N_F + 2) &= \sum_{i=1}^2 e_{Q_i}^2 a_s^2 \left[ A_{Qq}^{(2),\text{PS}}(N_F + 2, m_i^2) \delta_2 + \tilde{C}_{q,(2,L)}^{(2),\text{PS}}(N_F + 2) \right] \\ &+ a_s^3 \left[ \tilde{A}_{Qq}^{(3),\text{PS}}(N_F + 2) \delta_2 + \sum_{i=1}^2 e_{Q_i}^2 \left[ \tilde{C}_{q,(2,L)}^{(3),\text{PS}}(N_F + 2) \right. \right. \\ &\quad + A_{gq,Q}^{(2)}(N_F + 2) \tilde{C}_{g,(2,L)}^{(1)}(N_F + 2) \\ &\quad \left. \left. + A_{Qq}^{(2),\text{PS}}(N_F + 2) C_{q,(2,L)}^{(1),\text{NS}}(N_F + 2) \right] \right], \end{aligned} \quad (2.96)$$

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$$\begin{aligned}
\tilde{H}_{g,(2,L)}^S(N_F+2) &= \sum_{i=1}^2 e_{Q_i}^2 \left[ a_s \left[ A_{Qg}^{(1)}(N_F+2) \delta_2 + \tilde{C}_{g,(2,L)}^{(1)}(N_F+2) \right] \right. \\
&+ a_s^2 \left[ A_{Qg}^{(2)}(N_F+2) \delta_2 + A_{Qg}^{(1)}(N_F+2) C_{q,(2,L)}^{(1),\text{NS}}(N_F+2) \right. \\
&\quad \left. \left. + A_{gg,Q}^{(1)}(N_F+2) \tilde{C}_{g,(2,L)}^{(1)}(N_F+2) + \tilde{C}_{g,(2,L)}^{(2)}(N_F+2) \right] \right] \\
&+ a_s^3 \left[ \tilde{A}_{Qg}^{(3)}(N_F+2) \delta_2 + \sum_{i=1}^2 e_{Q_i}^2 \left[ A_{Qg}^{(2)}(N_F+2) C_{q,(2,L)}^{(1),\text{NS}}(N_F+2) \right. \right. \\
&\quad \left. \left. + A_{gg,Q}^{(2)}(N_F+2) \tilde{C}_{g,(2,L)}^{(1)}(N_F+2) \right. \right. \\
&\quad \left. \left. + A_{Qg}^{(1)}(N_F+2) \left\{ C_{q,(2,L)}^{(2),\text{NS}}(N_F+2) + \tilde{C}_{q,(2,L)}^{(2),\text{PS}}(N_F+2) \right\} \right. \right. \\
&\quad \left. \left. + A_{gg,Q}^{(1)}(N_F+2) \tilde{C}_{g,(2,L)}^{(2)}(N_F+2) + \tilde{C}_{g,(2,L)}^{(3)}(N_F+2) \right] \right]. \quad (2.97)
\end{aligned}$$

Here the symbol  $\delta_2$  takes the values

$$\delta_2 = \begin{cases} 1 & \text{for } F_2 \\ 0 & \text{for } F_L. \end{cases} \quad (2.98)$$

The double tilde in  $\tilde{\tilde{H}}_{q,(2,L)}^{\text{PS}}$  and  $\tilde{\tilde{H}}_{g,(2,L)}$  should not be interpreted as applying Eq. (2.90) twice. Instead, it is used to differentiate these Wilson coefficients from those of the single mass case, indicating now the required sum over charges as made explicit later in Eqs. (2.96,2.97).

Because of the coupling of the exchanged gauge boson to the heavy quark line in the case of the Wilson coefficients denoted by  $\tilde{\tilde{H}}$ , we have still to present the detailed structure of the 3-loop OMEs  $A_{ij}^{(3)}$  in this case. They consist of the two equal mass terms  $A_{ij}^{(3)}(m_1^2)$ ,  $A_{ij}^{(3)}(m_2^2)$  and the unequal mass term  $\tilde{A}_{ij}^{(3)}(m_1^2, m_2^2)$ ,

$$\tilde{A}_{ij}^{(3)}(m_1, m_2) = \bar{A}_{ij}^{(3)}(m_1, m_2) + \bar{A}_{ij}^{(3)}(m_2, m_1) \quad (2.99)$$

which is symmetric in  $m_1$  and  $m_2$ . The representation given in Eq. (2.99) is only relevant in the case of  $A_{Qg}^{(3)}$  and  $A_{Qg}^{(3),\text{PS}}$ . Here  $\bar{A}_{ij}^{(3)}(m_1, m_2)$  denotes the part for which the current couples to the fermion-loop of the heavy quark of mass  $m_1$ . This line is carrying the respective local operator. In general, the following representation holds

$$A_{ij}^{(3)}(m_1, m_2) = A_{ij}^{(3)}(m_1) + A_{ij}^{(3)}(m_2) + \tilde{A}_{ij}^{(3)}(m_1, m_2). \quad (2.100)$$

The charge-weighted OME is thus given by

$$\tilde{\tilde{A}}_{ij}^{(3)} = e_{Q_1}^2 A_{ij}^{(3)}(m_1) + e_{Q_2}^2 A_{ij}^{(3)}(m_2) + e_{Q_1}^2 \bar{A}_{ij}^{(3)}(m_1, m_2) + e_{Q_2}^2 \bar{A}_{ij}^{(3)}(m_2, m_1). \quad (2.101)$$

In the FFNS we can decompose the inclusive structure functions into contributions from light flavors and gluons and contributions from heavy quarks only

$$F_i(x, Q^2) = F_i^{\text{light}}(x, Q^2) + F_i^{\text{heavy}}(x, Q^2). \quad (2.102)$$

The contributions from the light flavors and gluons is essential given by Eq. (2.57). The heavy quark part of the structure functions is given by

$$\frac{1}{x} F_{(2,L)}^{\text{heavy}}(x, N_F + 2, Q^2, m_1^2, m_2^2) =$$

$$\begin{aligned}
 & \sum_{k=1}^{N_F} e_k^2 \left\{ L_{q,(2,L)}^{\text{NS}} \left( x, N_F + 2, \frac{Q^2}{\mu^2}, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \otimes [f_k(x, \mu^2, N_F) + f_{\bar{k}}(x, \mu^2, N_F)] \right. \\
 & \quad + \frac{1}{N_F} L_{q,(2,L)}^{\text{PS}} \left( x, N_F + 2, \frac{Q^2}{\mu^2}, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \otimes \Sigma(x, \mu^2, N_F) \\
 & \quad \left. + \frac{1}{N_F} L_{g,(2,L)}^{\text{S}} \left( x, N_F + 2, \frac{Q^2}{\mu^2}, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \otimes G(x, \mu^2, N_F) \right\} \\
 & + \tilde{H}_{q,(2,L)}^{\text{PS}} \left( x, N_F + 2, \frac{Q^2}{\mu^2}, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \otimes \Sigma(x, \mu^2, N_F) \\
 & + \tilde{H}_{g,(2,L)}^{\text{S}} \left( x, N_F + 2, \frac{Q^2}{\mu^2}, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \otimes G(x, \mu^2, N_F) . \tag{2.103}
 \end{aligned}$$

## 2.4. The Variable Flavor Number Scheme

From three loops onwards diagrams with both  $c$ - and  $b$ -quarks lead to power correction in  $\eta$  to the massive operator elements, which can manifest themselves in terms of higher transcendental functions. But even at the two loop level a consistent decoupling of both heavy quarks simultaneously give rise to two-mass effects from reducible contributions. One obtains the following transition relations decoupling both the charm and bottom contributions at high scales  $\mu^2 \gg m_1^2, m_2^2$  :

$$\begin{aligned}
 f_k(N_F + 2, N, \mu^2, m_1^2, m_2^2) + f_{\bar{k}}(N_F + 2, N, \mu^2, m_1^2, m_2^2) = \\
 A_{qq,Q}^{\text{NS}} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot [f_k(N_F, N, \mu^2) + f_{\bar{k}}(N_F, N, \mu^2)] \\
 + \frac{1}{N_F} A_{qq,Q}^{\text{PS}} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot \Sigma(N_F, N, \mu^2) \\
 + \frac{1}{N_F} A_{qg,Q} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot G(N_F, N, \mu^2), \tag{2.104}
 \end{aligned}$$

$$\begin{aligned}
 f_Q(N_F + 2, N, \mu^2, m_1^2, m_2^2) + f_{\bar{Q}}(N_F + 2, N, \mu^2, m_1^2, m_2^2) = \\
 A_{Qq}^{\text{PS}} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot \Sigma(N_F, N, \mu^2) \\
 + A_{Qg} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot G(N_F, N, \mu^2) . \tag{2.105}
 \end{aligned}$$

The flavor singlet, non-singlet and gluon densities for  $(N_F + 2)$  flavors are given by

$$\begin{aligned}
 \Sigma(N_F + 2, N, \mu^2, m_1^2, m_2^2) = & \left[ A_{qq,Q}^{\text{NS}} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + A_{qq,Q}^{\text{PS}} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right. \\
 & \left. + A_{Qq}^{\text{PS}} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right] \cdot \Sigma(N_F, N, \mu^2) \\
 & + \left[ A_{qg,Q} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + A_{Qg} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right] \cdot G(N_F, N, \mu^2) , \tag{2.106}
 \end{aligned}$$

$$\begin{aligned}
 \Delta_k(N_F + 2, N, \mu^2, m_1^2, m_2^2) = & f_k(N_F + 2, N, \mu^2, m_1^2, m_2^2) + f_{\bar{k}}(N_F + 2, N, \mu^2, m_1^2, m_2^2) \\
 & - \frac{1}{N_F + 2} \Sigma(N_F + 2, N, \mu^2, m_1^2, m_2^2) , \tag{2.107}
 \end{aligned}$$

## 2. Deep Inelastic Scattering

$$\begin{aligned}
G(N_F + 2, N, \mu^2, m_1^2, m_2^2) &= A_{gq,Q} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot \Sigma(N_F, N, \mu^2) \\
&+ A_{gg,Q} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot G(N_F, N, \mu^2). \tag{2.108}
\end{aligned}$$

Here  $f_{k(\bar{k})}(N_F), \Sigma(N_F)$  and  $G(N_F)$  denote the massless quarkonic parton densities. Note that in the above process the OMEs  $A_{ij}$  contain besides logarithmic corrections also power corrections in  $\eta$ . For general values of  $N$  the  $\eta$ -dependence is involved and requests at least generalized harmonic sums [240, 250] and binomially weighted generalized harmonic sums [241] as will be shown below in Section 7.

The presence of 2-mass terms in Eqs. (2.104-2.108) only allows to define the new parton densities at  $(N_F + 2)$  out of those at  $N_F$  at sufficiently high decoupling scales  $\mu^2 \gg m_1^2, m_2^2$  at 3-loop order, while up to 2-loop order, flavors can technically be decoupled one by one, if  $m_2^2 \gg m_1^2$ . However for the physical quark masses  $m_c^2/m_b^2 = \eta \sim 0.1$  this is hardly possible. Therefore the picture of an individual charm and bottom quark density does not hold from 3-loop order onwards. The quantities  $f_k + f_{\bar{k}}, \Sigma, \Delta_k$  and  $G$  are not affected, as they depend on all heavy quark masses in a symmetric way. The two-mass generalization (2.105) of the single mass case [180, 182], is a formal relation as it stands. It can be rewritten expressing the charm and bottom quark densities in the variable flavor scheme, still requesting

$$Q^2 \gg m_c^2 \quad \text{and} \quad Q^2 \gg m_b^2 \tag{2.109}$$

by

$$\begin{aligned}
f_c(N_F + 2, N, \mu^2, m_1^2, m_2^2) + f_{\bar{c}}(N_F + 2, N, \mu^2, m_1^2, m_2^2) &= \\
&\bar{A}_{Qq}^{\text{PS},c(b)} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot \Sigma(N_F, N, \mu^2) \\
&+ \bar{A}_{Qg}^{c(b)} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot G(N_F, N, \mu^2) \tag{2.110}
\end{aligned}$$

$$\begin{aligned}
f_b(N_F + 2, N, \mu^2, m_1^2, m_2^2) + f_{\bar{b}}(N_F + 2, N, \mu^2, m_1^2, m_2^2) &= \\
&\bar{A}_{Qq}^{\text{PS},b(c)} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot \Sigma(N_F, N, \mu^2) \\
&+ \bar{A}_{Qg}^{b(c)} \left( N, N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot G(N_F, N, \mu^2), \tag{2.111}
\end{aligned}$$

where

$$\bar{A}_{ij}^{c(b)} = A_{ij}^{(3)}(m_c) + \bar{A}_{ij}^{(3)}(m_c, m_b), \tag{2.112}$$

and  $\bar{A}_{ij}^{b(c)}$  is obtained by  $c \leftrightarrow b$ . Eq. (2.105) is the sum of Eqs. (2.110,2.111). The OME  $\bar{A}_{ij}^{(3)}(m_c, m_b)$  can be identified with the diagrams of the two-mass contribution where the operator sits on the charm quark line whereas for  $\bar{A}_{ij}^{(3)}(m_b, m_c)$  the operator sits on the bottom quark line. Up to next-to-leading order all ingredients for the VFNS are known and it is presented explicitly in Chapter 6. Chapter 7 is devoted to the calculation of the two-mass contributions to the OMEs  $A_{Qq}^{(3),\text{PS}}$  and  $A_{gg,Q}^{(3)}$  which are essential contributions for the VFNS at next-to-next-to-leading order. With the completion of these contributions only the single mass contributions to the OME  $A_{gg,Q}^{(3)}$  in momentum space and the OME  $A_{Qg}^{(3)}$  are missing.



### 3. Unpolarized Pure-Singlet Wilson Coefficients at NLO

The complete massive two-loop Wilson coefficients for deep-inelastic scattering corresponding to the structure functions  $F_2(x, Q^2)$  and  $F_L(x, Q^2)$  were only available in numerical form [168–170]<sup>1</sup> for a long time. Later the flavor non-singlet Wilson coefficients have been calculated analytically in [173, 179] in the tagged-flavor case and recalculated for the inclusive case [178] to obtain a representation consistent with the associated sum rules.

In this chapter the massive pure singlet two-loop Wilson coefficients are calculated analytically. Due to the corresponding graphs, the formulae are structurally the same for the charm and the bottom contributions. In the numerical illustrations we will concentrate on the charm contributions, considering the first three quarks as massless. The knowledge of the complete analytic expressions allows to derive important limiting cases such as the limit of large virtualities  $Q^2 \gg m^2$ ,  $m$  being the heavy quark mass, or the threshold expansion in a direct way. In the former case it is possible to derive systematic expansions in  $m^2/Q^2$  with coefficients represented in terms of harmonic polylogarithms, while the complete result depends on much more general functions. Harmonic polylogarithms can be easily calculated numerically [251–253]. Furthermore, they can be directly transformed to Mellin space [149, 150]. It has been observed numerically in Ref. [179] that the limit of large virtualities is approached beyond some process-dependent scale  $Q_0^2$ . The Wilson coefficient in this limit can be calculated with the help of massive operator matrix elements (OMEs) and massless Wilson coefficients, cf. [179]. It is important to prove this analytically. At three-loop order the massive Wilson coefficients are only known in the asymptotic region [1, 2, 182, 202, 254–261]. We also recalculate the corresponding massless two-loop Wilson coefficients given in [86, 129, 132, 135, 136, 138, 262, 263] before and compare to these results.

After the non-singlet contribution had been obtained [179], the analytic calculation of the massive pure singlet Wilson coefficient can be envisaged since the underlying Feynman graphs have only tree structures. However, adequate mathematical techniques to perform this task have only become available very recently. This includes the elimination of all functional relations in the final result and techniques to obtain a compact representation. The massive Wilson coefficient is given by a four-fold non-trivial phase space integral. Three of the integrals can be carried out using standard techniques. The integrand of the last integral is obtained as a polynomial of rational terms, logarithms and polylogarithms [264–266] with an involved argument structure. Therefore, the last integral is performed after determining the contributing irreducible structure of letters of the contributing iterated integrals, using the techniques described in [241, 267]. The Wilson coefficient can finally be obtained as a d'Alembertian integral over a finite alphabet. The analytic results allow to perform expansions in  $m^2/Q^2$  including power corrections, which is of particular importance for the structure function  $F_L(x, Q^2)$ . Here the corresponding expansion coefficients are then harmonic polylogarithms. Such a representation is easily envisaged for the two-loop non-singlet Wilson coefficients given in [178, 179], since there the whole Wilson coefficient depends at most on classical polylogarithms.

We also consider the limit  $Q^2 \gg m^2$  of the Wilson coefficient and compare with the results given in Refs. [179, 185, 260]. Furthermore, the threshold expansion of the Wilson coefficients are derived and numerical results are presented. In the present calculations, the packages FORM [198, 199], Sigma

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<sup>1</sup>Numerical results were also presented in [177].

### 3. Unpolarized Pure-Singlet Wilson Coefficients at NLO

[268, 269], `EvaluateMultiSums` [270, 271] and `HarmonicSums` [149, 150, 240, 272–275] have been used.

The chapter has the following structure. In Section 3.1 we first illustrate the asymptotic factorization using the example of the  $\mathcal{O}(\alpha_s)$  calculation. The corresponding scattering cross sections will be used in the two-loop massless and massive calculation later. In Section 3.2 the massless two-loop pure singlet Wilson coefficients are calculated. The mathematical method used to prepare for the last analytic integral in the massive case is described in Section 3.3 and in Section 3.4 we present the analytic results for the massive Wilson coefficients. The asymptotic and threshold expansions are derived in Section 3.5 and numerical results are presented in Section 3.6. Some technical aspects of the calculation are given in the Appendix D.

#### 3.1. Asymptotic cross section factorization

The massive Wilson coefficients are calculated by factorizing the *massless* initial states (quarks and gluons). In the unpolarized case and for longitudinal polarization the factorization is longitudinal, i.e. by setting  $p = zP, z \in [0, 1]$ . Here  $P$  denotes the incoming hadron momentum and  $p$  the quark momentum. In the transversal polarized case one has to use the covariant parton model [276], see [174, 277–279].

As an illustrative example we consider the unpolarized one-loop heavy flavor contribution to deep-inelastic scattering [163–166, 280]. As for all the massive Wilson coefficients, it can be written in three parts: the massive operator matrix element, the massless Wilson coefficient and a remainder part. The last one vanishes in the limit  $Q^2/m^2 \rightarrow \infty$  in the case of *asymptotic factorization*. A simple prediction on the structure of this term is not easily possible, but usually requires the calculation of the whole process followed by the expansion in  $m^2/Q^2$ . This term depends on the structure of the phase space and it is a process-dependent quantity. In Fig. 3.1 the contributing Feynman diagrams are shown.

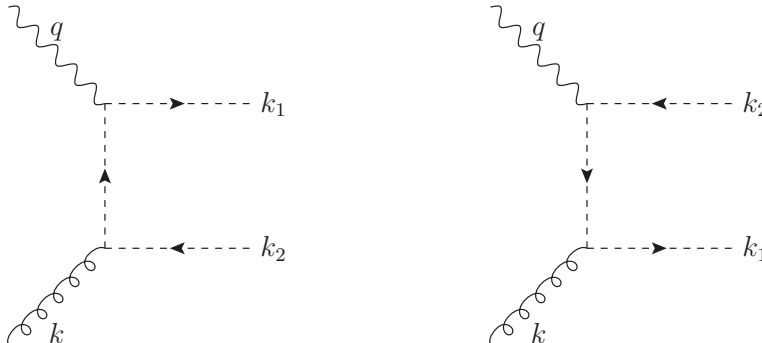


Figure 3.1.: Diagrams of the  $\mathcal{O}(\alpha_s)$  contributions to scattering cross section  $\gamma^* + g \rightarrow q + \bar{q}$ .

The massive Wilson coefficients have the following series representation

$$H_{2(L),i} \left( z, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) = \sum_{k=1}^{\infty} a_s^k H_{2(L),i}^{(k)} \left( z, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right), \quad (3.1)$$

where  $i$  denotes the incoming parton and  $2(L)$  refer to the associated structure functions. Since we also need the  $\mathcal{O}(\varepsilon)$  term of the LO result later on, we further define

$$H_{2(L),i}^{(1)} \left( z, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) = h_{2(L),i}^{(1)} + \varepsilon \bar{b}_{2(L),i}^{(1)}, \quad (3.2)$$

where we dropped the arguments of the coefficient functions for brevity.

Let us consider the leading order contribution for the process  $\gamma^* + g \rightarrow Q\bar{Q}$  as an example, cf. [163–166, 280]. In the following we use the variable

$$\beta = \sqrt{1 - \frac{4m^2}{Q^2} \frac{z}{1-z}}. \quad (3.3)$$

The Wilson coefficients  $H_{L,g}^{(1)}$  and  $H_{2,g}^{(1)}$  are given by

$$h_{L,g}^{(1)}\left(z, \frac{Q^2}{m^2}\right) = 16T_F \left[ \beta z(1-z) + 2\frac{m^2}{Q^2} z^2 \ln\left(\frac{1-\beta}{1+\beta}\right) \right] \theta(a-z), \quad (3.4)$$

$$\begin{aligned} h_{2,g}^{(1)}\left(z, \frac{Q^2}{m^2}\right) &= 8T_F \left\{ \beta \left[ -\frac{1}{2} + 4z(1-z) - 2\frac{m^2}{Q^2} z(1-z) \right] \right. \\ &\quad \left. + \left[ -\frac{1}{2} + z - z^2 + 2\frac{m^2}{Q^2} z(3z-1) + 4\left(\frac{m^2}{Q^2}\right)^2 z^2 \right] \ln\left(\frac{1-\beta}{1+\beta}\right) \right\} \\ &\quad \times \theta(a-z), \end{aligned} \quad (3.5)$$

with  $\theta(x)$  the Heaviside function and  $a = 1/(1 + 4m^2/Q^2)$ . The coefficients at  $\mathcal{O}(\varepsilon)$  read

$$\begin{aligned} \bar{b}_{L,g}^{(1)} &= T_F z(1-z) \left\{ 2(1-\beta^2) \left[ \mathbf{H}_0^2\left(\frac{1-\beta}{1+\beta}\right) - 2\mathbf{H}_0\left(\frac{1-\beta}{1+\beta}\right) [1 + \mathbf{H}_0 + \mathbf{H}_1 - 2\mathbf{H}_0(\beta)] \right] \right. \\ &\quad - 8 \left[ \beta(3 + \mathbf{H}_0 + \mathbf{H}_1 - 2\mathbf{H}_0(\beta)) + (1-\beta^2) \left[ \mathbf{H}_{0,1}\left(\frac{1-\beta}{1+\beta}\right) + [\ln(2) + \mathbf{H}_0(\beta) \right. \right. \right. \\ &\quad \left. \left. \left. - \mathbf{H}_{-1}(\beta)] \mathbf{H}_0\left(\frac{1-\beta}{1+\beta}\right) - \zeta_2 \right] \right] \right\} \theta(a-z), \end{aligned} \quad (3.6)$$

$$\begin{aligned} \bar{b}_{2,g}^{(1)} &= T_F \left\{ 2(1-z)(1-\beta^2) [\beta^2 - z(3 + \beta^2)] \mathbf{H}_0\left(\frac{1-\beta}{1+\beta}\right) - \frac{1}{2} \mathbf{H}_0^2\left(\frac{1-\beta}{1+\beta}\right) \right. \\ &\quad \times [3 - \beta^4 - 2z(5 - 2\beta^2 - \beta^4) + z^2(9 - 4\beta^2 - \beta^4)] + 2\beta[5 - 2\beta^2 \\ &\quad + 2z^2(12 - \beta^2) - 2z(13 - 2\beta^2)] - 2 \left[ 3 - \beta^4 - 2z(5 - 2\beta^2 - \beta^4) \right. \\ &\quad \left. + z^2(9 - 4\beta^2 - \beta^4) \right] \left[ -\mathbf{H}_{0,1}\left(\frac{1-\beta}{1+\beta}\right) - [\ln(2) + \mathbf{H}_0(\beta) - \mathbf{H}_0(1+\beta)] \mathbf{H}_0\left(\frac{1-\beta}{1+\beta}\right) + \zeta_2 \right] \\ &\quad \left. + \left[ 2\beta(2 - \beta^2 + z^2(9 - \beta^2) - 2z(5 - \beta^2)) + [3 - \beta^4 - 2z(5 - 2\beta^2 - \beta^4) \right. \right. \\ &\quad \left. \left. + z^2(9 - 4\beta^2 - \beta^4)] \mathbf{H}_0\left(\frac{1-\beta}{1+\beta}\right) \right] [\mathbf{H}_1 + \mathbf{H}_0 - 2\mathbf{H}_0(\beta)] \right\} \theta(a-z). \end{aligned} \quad (3.7)$$

We refer to the harmonic polylogarithms [151] as introduced in Appendix C.4. Here and in the following chapter we use the abbreviation  $\mathbf{H}_{\bar{a}}(z) \equiv \mathbf{H}_{\bar{a}}$  if not stated otherwise.

The expansion for large virtualities  $Q^2 \gg m^2$  is given by

$$H_{L,g}^{(1)}\left(z, \frac{Q^2}{m^2}\right) = 16T_F \left\{ z(1-z) - 2\frac{m^2}{Q^2} z^2 \left[ \ln\left(\frac{Q^2}{m^2}\right) + 1 - \mathbf{H}_1 - \mathbf{H}_0 \right] + \mathcal{O}\left(\left(\frac{m^2}{Q^2}\right)^2\right) \right\}, \quad (3.8)$$

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$$\begin{aligned}
H_{2,g}^{(1)}\left(z, \frac{Q^2}{m^2}\right) &= 4T_F \left\{ -1 + 8z(1-z) + [z^2 + (1-z)^2] \left[ \ln\left(\frac{Q^2}{m^2}\right) - H_1 - H_0 \right] \right. \\
&\quad \left. + 4\frac{m^2}{Q^2} \left[ -z(1+2z) + (1-3z)z \left[ \ln\left(\frac{Q^2}{m^2}\right) - H_1 - H_0 \right] \right] + \mathcal{O}\left(\left(\frac{m^2}{Q^2}\right)^2\right) \right\}
\end{aligned} \tag{3.9}$$

for  $z \in [0, a]$ .

In the asymptotic case, one has [179]

$$H_{L,g}^{(1)}\left(z, \frac{Q^2}{m^2}\right) = \tilde{C}_{g,L}^{(1)}(N_F + 1), \tag{3.10}$$

$$H_{2,g}^{(1)}\left(z, \frac{Q^2}{m^2}\right) = A_{Qg}^{(1)}(N_F + 1) + \tilde{C}_{g,2}^{(1)}(N_F + 1), \tag{3.11}$$

using the definition

$$\tilde{f}(N_F) = \frac{f(N_F)}{N_F}, \quad \hat{f}(N_F + 1) = f(N_F + 1) - f(N_F). \tag{3.12}$$

Note that Eqs. (3.10, 3.11) hold for  $z \in [0, 1]$ . Here  $C_{g,2(L)}^{(1)}$  denote the massless two-loop Wilson coefficients and  $A_{Qg}^{(1)}$  the massive one-loop operator matrix element (OME) with external gluons [179, 185, 260]

$$A_{Qg}^{(1)} = -4T_F [z^2 + (1-z)^2] \ln\left(\frac{m^2}{\mu^2}\right). \tag{3.13}$$

The massless one-loop Wilson coefficients read [94, 128, 131]

$$\tilde{C}_{g,L}^{(1)} = 16T_F z(1-z), \tag{3.14}$$

$$\begin{aligned}
\tilde{C}_{g,2}^{(1)} &= 4T_F [z^2 + (1-z)^2] \ln\left(\frac{Q^2}{\mu^2}\right) \\
&\quad - 4T_F \{1 - 8z(1-z) + [z^2 + (1-z)^2] [H_1 + H_0]\},
\end{aligned} \tag{3.15}$$

where

$$\hat{P}_{qg}(z) = 8T_F [z^2 + (1-z)^2] \tag{3.16}$$

is a one-loop splitting function [89, 90]<sup>2</sup>.

It can now be seen that the massive Wilson coefficients can be decomposed in terms of the part obtained at large virtualities  $Q^2 \gg m^2$ , Eqs. (3.10,3.11), consisting of massive OMEs and massless Wilson coefficients, and a remainder part vanishing in the limit  $Q^2/m^2 \rightarrow \infty$ . Whenever this is the case one calls the respective process *asymptotically factorizing*. The factorization scale  $\mu$  cancels in the cross sections in Eqs. (3.10, 3.11) since they are free of collinear singularities. As a peculiarity in this case, the massive OME only contributes to the pure logarithmic term. This, however, is due to its vanishing constant part and is generally not the case.

Numerically it is interesting to see from which value of  $Q_0^2/m^2$  onward the asymptotic representation holds, say at the accuracy of  $\mathcal{O}(2\%)$  or better, cf. [178, 179] and Section 3.6.

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<sup>2</sup>For earlier references in QED, see [224].

### 3.2. The massless Wilson coefficients

The massless pure singlet Wilson coefficients obey the expansion

$$C_{2(L)}^{\text{PS}} \left( z, \frac{Q^2}{\mu^2} \right) = \delta(1-z)\delta_2 + \sum_{k=1}^{\infty} a_s^k C_{2(L)}^{(k),\text{PS}} \left( z, \frac{Q^2}{\mu^2} \right), \quad (3.17)$$

with  $\delta_2 = 1$  for  $C_2^{\text{PS}}$  and  $\delta_2 = 0$  for  $C_L^{\text{PS}}$ . We will identify both the factorization scale  $\mu_F$  and the renormalization scale  $\mu_R$  with  $\mu$ .

In the following we also recalculate the massless Wilson coefficients  $C_L^{(2),\text{PS}}$  and  $C_2^{(2),\text{PS}}$  as a limiting case of the present massive calculation. They have been computed in Refs. [86, 129, 132, 135, 136, 138, 262] before.

The unrenormalized Wilson coefficients  $\mathcal{F}_{L(2),q}$  are related to the hadronic tensor of deeply inelastic scattering in the partonic sub-system,  $\hat{W}_{\mu\nu}$ , by

$$\mathcal{F}_{L,q} = -\frac{2q^2}{(p \cdot q)^2} p_\mu p_\nu \hat{W}_{\mu\nu}, \quad (3.18)$$

$$\mathcal{F}_{2,q} = -\frac{2}{d-2} \left[ \hat{W}_\mu^\mu + (d-1) \frac{q^2}{(p \cdot q)^2} p^\mu p^\nu \hat{W}_{\mu\nu} \right]. \quad (3.19)$$

Here  $p$  denotes the incoming parton momentum and  $q$  the space-like momentum of the virtual photon with  $q^2 = -Q^2$ .

In the massive case we will also consider the Wilson coefficient

$$\mathcal{F}_{1,q} = -2\hat{W}_\mu^\mu \quad (3.20)$$

as a subsidiary function in order to avoid redundancies in the calculation. Note that this Wilson coefficient does not correspond to the structure function  $F_1$ , cf. [224].

The following expressions will be given in Mellin- $N$  space. The unrenormalized Wilson coefficients  $\mathcal{F}_{L(2),q}^{(2),\text{PS}}$  are given by [131]

$$\mathcal{F}_{L,q}^{(2),\text{PS}} = N_F \hat{a}_s^2 S_\varepsilon^2 \left( \frac{Q^2}{\mu^2} \right)^\varepsilon \left[ \frac{1}{\varepsilon} P_{gq}^{(0)} c_{L,g}^{(1)} + c_{L,q}^{(2),\text{PS}} + P_{gq}^{(0)} a_{L,g}^{(1)} \right], \quad (3.21)$$

$$\mathcal{F}_{2,q}^{(2),\text{PS}} = N_F \hat{a}_s^2 S_\varepsilon^2 \left( \frac{Q^2}{\mu^2} \right)^\varepsilon \left[ \frac{1}{\varepsilon^2} \frac{1}{2} P_{qg}^{(0)} P_{gq}^{(0)} + \frac{1}{\varepsilon} \left( \frac{1}{2} P_{qq}^{(1),\text{PS}} + P_{gq}^{(0)} c_{2,g}^{(1)} \right) + c_{2,q}^{(2),\text{PS}} + P_{gq}^{(0)} a_{2,g}^{(1)} \right], \quad (3.22)$$

with  $\hat{a}_s$  the unrenormalized coupling constant and the spherical factor  $S_\varepsilon$ , see Eqs. (G.17). We work in the  $\overline{\text{MS}}$ -scheme and set  $S_\varepsilon = 1$  at the end of the calculation. Here the factors of  $1/2$  in Eq. (3.22) emerge since for the splitting into the upper quark-antiquark pair, the quarks are produced correlated. Since the pure singlet contributions start at  $\mathcal{O}(a_s^2)$  only, the renormalized Wilson coefficients  $C_{L(2)}^{(2),\text{PS}}$  are obtained after mass factorization

$$\mathcal{F}_{L,q}^{(2),\text{PS}} = C_{L,q}^{(2),\text{PS}} + \Gamma_{gq}^{(0)} C_{L,q}^{(2),\text{PS}}, \quad (3.23)$$

$$\mathcal{F}_{2,q}^{(2),\text{PS}} = C_{2,q}^{(2),\text{PS}} + \frac{1}{2} \Gamma_{qq}^{(1),\text{PS}} C_{2,q}^{(2),\text{PS}} + \Gamma_{gq}^{(0)} C_{2,g}^{(1)}, \quad (3.24)$$

with

$$\Gamma_{gq}^{(0)} = \hat{a}_s S_\varepsilon \left( \frac{\mu_F^2}{\mu^2} \right)^{\varepsilon/2} \frac{1}{\varepsilon} P_{gq}^{(0)}, \quad (3.25)$$

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$$\Gamma_{qq}^{(1),\text{PS}} = \hat{a}_s^2 S_\varepsilon^2 \left( \frac{\mu_F^2}{\mu^2} \right)^\varepsilon \left[ \frac{1}{\varepsilon^2} P_{qq}^{(0)} P_{qq}^{(0)} + \frac{1}{\varepsilon} P_{qq}^{(1),\text{PS}} \right]. \quad (3.26)$$

In  $z$ -space the functions in Eqs. (3.21, 3.22) read

$$a_{L,g}^{(1)} = -8T_F z(1-z) [3 + H_1 + H_0], \quad (3.27)$$

$$a_{2,g}^{(1)} = T_F \left\{ [z^2 + (1-z)^2] (H_1 + H_0)^2 + 2(1-8z(1-z))(H_1 + H_0) - 3[z^2 + (1-z)^2] \zeta_2 + 6 - 44z(1-z) \right\}, \quad (3.28)$$

see as well Eqs. (3.14, 3.15) for  $\mu^2 = Q^2$ . The splitting functions are

$$P_{gg}^{(0)} = N_F \hat{P}_{gg}^{(0)}, \quad (3.29)$$

$$P_{gq}^{(0)} = 4C_F \frac{1 + (1-z)^2}{z}, \quad (3.30)$$

$$P_{qq}^{(1),\text{PS}} = 16C_F T_F N_F \left[ \frac{20}{9} \frac{1}{z} - 2 + 6z - 4H_0 + z^2 \left( \frac{8}{3} H_0 - \frac{56}{9} \right) + (1+z) (5H_0 - H_0^2) \right]. \quad (3.31)$$

The massless Wilson coefficients  $C_L^{(2),\text{PS}}$  and  $C_2^{(2),\text{PS}}$  are thus given by

$$C_L^{(2),\text{PS}} \left( z, \frac{Q^2}{\mu_F^2} \right) = -32C_F T_F N_F \left\{ \left[ zH_0 + \frac{1}{3} \left( 3 - 2z^2 - \frac{1}{z} \right) \right] \ln \left( \frac{Q^2}{\mu_F^2} \right) + \frac{(1-z)(1-2z+10z^2)}{9z} - (1+z)(1-2z)H_0 - zH_0^2 + \frac{(1-z)(1-2z-2z^2)}{3z} H_1 - zH_{0,1} + z\zeta_2 \right\}, \quad (3.32)$$

$$C_2^{(2),\text{PS}} \left( z, \frac{Q^2}{\mu_F^2} \right) = C_F T_F N_F \left\{ \left[ 8(1+z)H_0 + \frac{4}{3} \left( 3 - 4z^2 - 3z + \frac{4}{z} \right) \right] \ln^2 \left( \frac{Q^2}{\mu_F^2} \right) + \left[ 16(1+z)[-H_{0,1} + \zeta_2 - H_0^2] + 32z^2 H_0 - \frac{8}{3} \left( 3 - 4z^2 - 3z + \frac{4}{z} \right) H_1 - \frac{16}{9} \left( 39 + 4z^2 - 30z - \frac{13}{z} \right) \right] \ln \left( \frac{Q^2}{\mu_F^2} \right) + \frac{4(1-z)(172 + 409z - 224z^2)}{27z} + \frac{16}{9} (63 - 33z - 16z^2) H_0 - \frac{32(1+z)^3 H_{-1} H_0}{3z} - \frac{2}{3} (3 - 45z + 32z^2) H_0^2 + \frac{20}{3} (1+z) H_0^3 + \left[ -\frac{16(1-z)(13 - 26z + 4z^2)}{9z} + \frac{8(4 + 3z - 6z^2 - 4z^3)}{3z} H_0 \right] H_1 + \frac{4(4 + 3z - 4z^3) H_1^2}{3z} + \left[ -\frac{8(1+2z)(4 - 5z + 4z^2)}{3z} + 16(1+z)H_0 \right] H_{0,1} + \frac{32(1+z)^3 H_{0,-1}}{3z} + 16(1+z)H_{0,1,1} - \left[ \frac{32(1+3z^2 - 3z^3)}{3z} + 32(1+z)H_0 \right] \zeta_2 - 16(1+z)\zeta_3 \right\}. \quad (3.33)$$

We agree with the results given in [86, 263] and note a typo in [129], Eq. (13), where the next-to-last term should read  $(448/27)x^2$ . In Appendix D.1 we present details of the calculation in the massless case.

The massless two-loop pure singlet contribution to the structure functions  $F_{2(L)}$  for pure virtual photon exchange is given by

$$F_{2(L)}^{(2),\text{PS}}(x, Q^2) = a_s^2(Q^2) Q_H^2 x C_{2(L)}^{\text{PS},(2)} \left( \frac{Q^2}{\mu^2}, x \right) \otimes \Sigma(x, \mu^2), \quad (3.34)$$

where  $\mu$  denotes the factorization scale,  $Q_H = 2/3$  for charm and  $Q_H = -1/3$  for bottom, and

$$\Sigma(x, \mu^2) = \sum_{k=1}^3 [q_k(x, \mu^2) + \bar{q}_k(x, \mu^2)] \quad (3.35)$$

denotes the quark singlet distribution for three light quarks.

### 3.3. Systematic integration in the massive case

We want to express the heavy Wilson coefficients  $H_{2(L)}^{(2),\text{PS}}$  in terms of a minimal number of special functions. In the case of single scale quantities, various methods have been worked out in the past to achieve this; for a recent survey see [281]. In the present case, we deal with a two-scale process, since the Wilson coefficients depend on  $z$  and  $m^2/Q^2$  in a non-factorizing way. The complete massive Wilson coefficients are represented in terms of four non-trivial integrals. The parametrization of the phase space is given in Appendix D. The first three integrations are evaluated in terms of logarithms and polylogarithms at various complex arguments involving square-roots and trigonometric functions. What remains is a one-fold integral with respect to the last integration variable  $x$ , cf. Appendix D.1, that also depends on the parameters  $z$  and  $\beta$ . The overall aim is to write this integral in terms of nested integrals. To this end, we first write its integrand in terms of nested integrals. We apply the change of integration variables

$$w = \beta\sqrt{x}. \quad (3.36)$$

In addition, we introduce the quantity

$$k := \frac{\sqrt{z}}{\sqrt{1 - (1-z)\beta^2}}, \quad (3.37)$$

which satisfies  $\sqrt{z} < k < 1$ . We use it to express  $\beta$  as  $\frac{\sqrt{k^2 - z}}{k\sqrt{1-z}}$ . Altogether, the integrand is then an expression in terms of  $z$ ,  $k$ , and  $w$  as well as logarithms and dilogarithms with arguments expressed in terms of square-roots involving these quantities.

Next, we eliminate redundancies among square-root expressions to express the integrand using only the roots  $\sqrt{1-k^2}$ ,  $\sqrt{1-w^2}$ , and  $\sqrt{1-k^2w^2}$ . In order to facilitate the conversion of the logarithms and dilogarithms appearing in the integrand to nested integrals, we exploit the argument relations

$$\ln(z) = \ln(-z) + i\pi \quad \text{for } z < 0 \quad (3.38)$$

$$\text{Li}_2(z) = -\text{Li}_2\left(\frac{1}{z}\right) - \frac{1}{2} \ln(z)^2 - i\pi \ln(z) + 2\zeta(2) \quad \text{for } z > 1 \quad (3.39)$$

to avoid arguments on branch cuts.

After these pre-processing steps, all the following steps for computing the integral are done by the code [282] in `Mathematica`, which also uses the routine `DSolveRational` of the package `HolonomicFunctions` [283]; see [267, 284] for the general theory underlying [282]. We also refer to

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[285] for the simpler case when no singularities are present at the endpoints of integration, which, however, does not apply here.

First, the logarithms and dilogarithms are converted to nested integrals, which is based on repeated differentiation followed by expressing the integrands of these nested integrals in the form developed in (3.16)–(3.19) of [241]. In fact, a generalized version of those forms is used to avoid the necessity of introducing new square-roots in terms of  $z$  and  $k$  in addition to  $\sqrt{1-k^2}$  above. Then, a normal form of the integrand is computed. This affects all parts of the representation, also those that do not depend on  $t$ . For the nested integrals we use the shuffle relations [286] and also for their coefficients we compute normal forms in terms of the logarithms and square-roots.

As a result, we obtain a representation of the integrand as a linear combination of nested integrals evaluated at  $w$  whose integrands also depend on  $z$  and  $k$ . Their coefficients only contain  $z$ ,  $k$ ,  $w$ ,  $\sqrt{1-w^2}$ ,  $\sqrt{1-k^2w^2}$ ,  $\ln(z)$ ,  $\ln(1-z)$ ,  $\ln(k+z)$ , and  $\ln(k-z)$ . The root  $\sqrt{1-k^2}$ , as well as all other logarithms and dilogarithms depending on  $z$  and  $k$ , do not appear in this representation anymore. Moreover, since both the integrand as a whole and all integrands of the nested integrals in its representation are real, all complex expressions drop out of the coefficients as well and we have a completely real representation. This is ensured since the integrands in (3.16)–(3.19) of [241], and also their generalization used here, are designed such that the corresponding nested integrals all are linearly independent.

Finally, the integral over  $w$  from 0 to  $\beta$  is computed as a linear combination of nested integrals evaluated at  $\beta$ , again in normal form. Like before, their integrands also depend on  $z$  and  $k$  and their coefficients only contain  $z$ ,  $k$ ,  $w$ ,  $\sqrt{1-w^2}$ ,  $\sqrt{1-k^2w^2}$ ,  $\ln(z)$ ,  $\ln(1-z)$ ,  $\ln(k+z)$ , and  $\ln(k-z)$ .

The following letters contribute in the present case:

$$f_{w_1}(t) = \frac{1}{1-kt}, \quad (3.40)$$

$$f_{w_2}(t) = \frac{1}{1+kt}, \quad (3.41)$$

$$f_{w_3}(t) = \frac{1}{\beta+t}, \quad (3.42)$$

$$f_{w_4}(t) = \frac{1}{\beta-t}, \quad (3.43)$$

$$f_{w_5}(t) = \frac{1}{k-z-(1-z)kt}, \quad (3.44)$$

$$f_{w_6}(t) = \frac{1}{k+z-(1-z)kt}, \quad (3.45)$$

$$f_{w_7}(t) = \frac{1}{k-z+(1-z)kt}, \quad (3.46)$$

$$f_{w_8}(t) = \frac{1}{k+z+(1-z)kt}, \quad (3.47)$$

$$f_{w_9}(t) = \frac{t}{k^2(1-t^2(1-z^2))-z^2}, \quad (3.48)$$

$$f_{w_{10}}(t) = \frac{1}{t\sqrt{1-t^2}\sqrt{1-k^2t^2}}, \quad (3.49)$$

$$f_{w_{11}}(t) = \frac{t}{\sqrt{1-t^2}\sqrt{1-k^2t^2}}, \quad (3.50)$$

$$f_{w_{12}}(t) = \frac{t}{\sqrt{1-t^2}\sqrt{1-k^2t^2}(k^2(1-t^2(1-z^2))-z^2)}. \quad (3.51)$$



The set of letters

$$\mathfrak{A} = \left\{ \frac{1}{t-a} \mid a \in \mathbb{C} \right\} \quad (3.52)$$

span the Kummer-Poincaré iterated integrals [287, 288] defined as

$$\mathbf{K}_{b,\bar{a}}(z) = \int_0^z dy f_b(y) \mathbf{K}_{\bar{a}}(y), \quad \mathbf{K}_\emptyset = 1, \quad f_c \in \mathfrak{A}. \quad (3.53)$$

The letter  $f_{w_9}$  can be rewritten into Kummer-Poincaré letters [287, 288], which we, however, avoid here. Some of the above letters contain the elliptic letter

$$\frac{1}{\sqrt{1-t^2}} \frac{1}{\sqrt{1-k^2t^2}} \quad (3.54)$$

as a factor. Therefore, one expects that in iterated integrals the incomplete elliptic integrals of the 1st, 2nd, and 3rd kind

$$F(x; k) = \int_0^x dt \frac{1}{\sqrt{1-t^2} \sqrt{1-k^2t^2}}, \quad (3.55)$$

$$E(x; k) = \int_0^x dt \frac{\sqrt{1-k^2t^2}}{\sqrt{1-t^2}}, \quad (3.56)$$

$$\Pi(n; x|k) = \int_0^x dt \frac{1}{1-nt^2} \frac{\sqrt{1-kt^2}}{\sqrt{1-t^2}}, \quad (3.57)$$

cf. [191, 289], are emerging, over which further Kummer-Poincaré letters are iterated. We call iterated integrals of this type *Kummer-elliptic* integrals. Their alphabet is

$$\begin{aligned} \mathfrak{A}' &= \mathfrak{A} \cup \left\{ \frac{1}{\sqrt{1-t^2} \sqrt{1-k^2t^2}}, \frac{t}{\sqrt{1-t^2} \sqrt{1-k^2t^2}}, \frac{\sqrt{1-k^2t^2}}{\sqrt{1-t^2}} \right\} \\ &\cup \left\{ \frac{1}{(t-a) \sqrt{1-t^2} \sqrt{1-k^2t^2}} \mid a \in \mathbb{C} \setminus \{\pm 1, \pm \frac{1}{k}\} \right\}. \end{aligned} \quad (3.58)$$

Note that integrals of depth 1 over the letters  $f_{w_1}$  to  $f_{w_{12}}$  are (poly)logarithmic, since one may change variables  $t \rightarrow \sqrt{t}$ , cf. Eqs. (3.48–3.51).

Yet Kummer-elliptic integrals appear in the iterated case. Therefore, iterated integrals of depth 2 formed out of some of these letters will form results containing incomplete elliptic integrals in part. These iterative integrals cannot be reduced to the Kummer-Poincaré iterated integrals for general values of  $k$ . As also the incomplete elliptic integrals, they belong to the d'Alembert class, unlike the complete elliptic integrals [191, 289], which also appear in various higher order calculations, cf. e.g. [290–297], as letters in other iterated integrals.

### 3.4. The massive Wilson coefficients

The unrenormalized two-loop massive pure singlet Wilson coefficients  $\mathcal{H}_{i,q}$  with  $i = 1, 2, L$ , see also Eq. (3.20), are given in Mellin space by

$$\mathcal{H}_{i,q}^{(2),\text{PS}} = \hat{a}_s^2 S_\varepsilon^2 \left( \frac{Q^2}{\mu^2} \right)^\varepsilon \left[ \frac{1}{\varepsilon} P_{gq}^{(0)} h_{i,g}^{(1)} + C_{i,q}^{(2),\text{PS},Q} + P_{gq}^{(0)} \bar{b}_{i,g}^{(1)} \right]. \quad (3.59)$$

The functions  $h_{1,g}^{(1)}$  and  $\bar{b}_{1,g}^{(1)}$  are given by

$$h_{1,g}^{(1)} = 2h_{2,g}^{(1)} - 3h_{L,q}^{(1)} \quad (3.60)$$

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$$\bar{b}_{1,g}^{(1)} = h_{2,g}^{(1)} - h_{L,q}^{(1)} + 2\bar{b}_{2,g}^{(1)} - 3\bar{b}_{L,q}^{(1)}. \quad (3.61)$$

Since the two heavy quarks do not induce collinear divergences the mass factorization in the massive case reads

$$\mathcal{H}_{i,q}^{(2),\text{PS}} = H_{i,q}^{(2),\text{PS}} + \Gamma_{gq} \otimes H_{i,g}^{(1)}. \quad (3.62)$$

Therefore, we find

$$\begin{aligned} H_{i,q}^{(2),\text{PS}} &= \hat{a}_s^2 S_\varepsilon^2 \left\{ \left( \frac{Q^2}{\mu^2} \right)^\varepsilon \left[ \frac{1}{\varepsilon} P_{gq}^{(0)} h_{i,g}^{(1)} + C_{i,q}^{(2),\text{PS},Q} + P_{gq}^{(0)} \bar{b}_{i,g}^{(1)} \right] \right. \\ &\quad \left. - \left( \frac{\mu_F^2}{\mu^2} \right)^{\varepsilon/2} \left( \frac{Q^2}{\mu^2} \right)^{\varepsilon/2} \left[ \frac{1}{\varepsilon} P_{gq}^{(0)} h_{i,g}^{(1)} + P_{gq}^{(0)} \bar{b}_{i,g}^{(1)} \right] \right\}. \end{aligned} \quad (3.63)$$

Identifying the renormalization and factorization scale,  $\mu = \mu_F$ , we finally obtain

$$\begin{aligned} H_{i,q}^{(2),\text{PS}} &= a_s^2 \left[ \frac{1}{2} P_{gq}^{(0)} h_{i,g}^{(1)} \ln \left( \frac{Q^2}{\mu_F^2} \right) + C_{i,q}^{(2),\text{PS},Q} \right] + \mathcal{O}(\varepsilon) \\ &= a_s^2 \left[ \frac{1}{2} P_{gq}^{(0)} h_{i,g}^{(1)} \ln \left( \frac{m^2}{\mu_F^2} \right) - \frac{1}{2} P_{gq}^{(0)} h_{i,g}^{(1)} \ln \left( \frac{m^2}{Q^2} \right) + C_{i,q}^{(2),\text{PS},Q} \right] + \mathcal{O}(\varepsilon). \end{aligned} \quad (3.64)$$

Note that in the pure singlet case the coupling constant is not renormalized at two-loop order. To express our final result in terms of iterated integrals we refer to the letters given in Section 3.3, supplemented by the letters spanning the harmonic polylogarithms, cf. Eqs. (C.34-C.35); for Eqs. (3.65) and (3.66) we use the shorthand notation  $H_{\vec{a}}(\beta) \equiv H_{\vec{a}}$ . One obtains

$$\begin{aligned} H_{L,q}^{(2),\text{PS}} &= C_{FTF} \left\{ -\frac{8P_1}{3z} \left\{ k \left[ H_{w_1}^2 - H_{w_2}^2 + (1-z)(H_{w_5,w_1} + H_{w_6,w_2} - H_{w_7,w_2} \right. \right. \right. \\ &\quad \left. \left. - H_{w_8,w_1} - H_{w_5}H_{w_1} + H_{w_8}H_{w_1} - H_{w_6}H_{w_2} + H_{w_7}H_{w_2} \right] + 2(H_{w_1,w_4} + H_{w_2,w_4} + H_{w_3,w_1} \right. \\ &\quad \left. + H_{w_3,w_2}) - (2H_{w_3} - 6\ln(k) + \ln(1-k^2) - \ln(k^2-z^2) + 2\ln(k^2-z)) [H_{w_1} \right. \\ &\quad \left. + H_{w_2}] \right\} - \frac{16(1-z)\beta P_2}{3z} \ln(k^2-z^2) - \frac{16(1-z)\beta P_3}{9k^2z} + \frac{8(1-k^2)(1-z)P_4}{3k^4z} [H_{w_5,0} \\ &\quad - H_{w_6,0} + H_{w_7,0} - H_{w_8,0} - (H_{w_5} - H_{w_6} + H_{w_7} - H_{w_8})H_0] + \frac{16(1-k^2)P_4}{3k^4z} (H_{w_1} \\ &\quad + H_{w_2})H_0 + \frac{32P_5}{3k^2} (H_{-1}H_1 - 2H_{-1,1}) + \frac{32P_6}{3k^4z} (H_{w_1,0} + H_{w_2,0}) + \frac{16P_7}{3k^4} (H_1H_{w_1} \\ &\quad - H_{-1}H_{w_2}) + \frac{16P_8}{3k^4} (H_1H_{w_2} - H_{-1}H_{w_1}) - \frac{64P_9}{3k^2z\beta} H_{w_3} - \frac{16(1-k^2)(1-z^2)P_{10}}{3k^2} [H_{w_9,1} \\ &\quad + H_{w_9,-1} - (1-z)k(H_{w_9,w_5} + H_{w_9,w_6} + H_{w_9,w_7} + H_{w_9,w_8})] - \frac{16P_{11}}{3k^2} (H_1^2 - H_{-1}^2) \\ &\quad - \frac{(1-z)P_{12}}{3z^{3/2}k^3} [H_{w_{10},w_5} - H_{w_{10},w_6} + H_{w_{10},w_7} - H_{w_{10},w_8} - k(H_{w_5,w_{11}} + H_{w_6,w_{11}} + H_{w_7,w_{11}} \\ &\quad + H_{w_8,w_{11}}) + k(H_{w_5} + H_{w_6} + H_{w_7} + H_{w_8})H_{w_{11}} - \frac{2}{1-z}(H_{w_{10},w_1} + H_{w_{10},w_2})] \\ &\quad + \frac{4(1+k)(1-z)P_{13}}{3k^4} (H_{w_6,-1} - H_{w_8,1} + H_{w_8}H_1 - H_{w_6}H_{-1}) \\ &\quad + \frac{4(1-k)(1-z)P_{14}}{3k^4} (H_{w_5,-1} - H_{w_7,1} + H_{w_7}H_1 - H_{w_5}H_{-1}) + \frac{8P_{15}}{3k^4z} (H_{w_1,1} - H_{w_2,-1}) \end{aligned}$$

$$\begin{aligned}
 & -\frac{4(1-z)P_{16}}{3k^4}(\mathbb{H}_{w_6,1} - \mathbb{H}_{w_8,-1} - \mathbb{H}_{w_6}\mathbb{H}_1 + \mathbb{H}_{w_8}\mathbb{H}_{-1}) - \frac{4(1-z)P_{17}}{3k^4}(\mathbb{H}_{w_5,1} - \mathbb{H}_{w_7,-1} \\
 & - \mathbb{H}_{w_5}\mathbb{H}_1 + \mathbb{H}_{w_7}\mathbb{H}_{-1}) - \frac{2(1-k^2)P_{18}}{3\sqrt{z}k^3} \left[ \mathbb{H}_{w_{12},1} + \mathbb{H}_{w_{12},-1} + (1-z)k(\mathbb{H}_{w_5,w_{12}} + \mathbb{H}_{w_6,w_{12}} \right. \\
 & \left. + \mathbb{H}_{w_7,w_{12}} + \mathbb{H}_{w_8,w_{12}}) - (1-z)k(\mathbb{H}_{w_5} + \mathbb{H}_{w_6} + \mathbb{H}_{w_7} + \mathbb{H}_{w_8})\mathbb{H}_{w_{12}} \right] - \frac{8P_{19}}{3k^4z}(\mathbb{H}_{w_1,-1} \\
 & - \mathbb{H}_{w_2,1}) + \frac{2P_{20}}{9k^2z(1-k\beta)}\mathbb{H}_{w_1} - \frac{2P_{21}}{9k^2z(1+k\beta)}\mathbb{H}_{w_2} + \frac{(1-z)P_{22}}{3k^3z(k(z-2)+z)(1-k\beta)}\mathbb{H}_{w_5} \\
 & + \frac{2P_{23}}{9k^4z(k^2(z-2)^2-z^2)}\mathbb{H}_1 - \frac{2P_{24}}{9k^4z(k^2(z-2)^2-z^2)}\mathbb{H}_{-1} \\
 & - \frac{(1-z)P_{25}}{3k^3z(k(z-2)-z)(1+k\beta)}\mathbb{H}_{w_6} + \frac{(1-z)P_{26}}{3k^3z(k(z-2)+z)(1+k\beta)}\mathbb{H}_{w_7} \\
 & + \frac{(1-z)P_{27}}{3k^3z(k(z-2)-z)(1-k\beta)}\mathbb{H}_{w_8} - 32(1-z)^2z(\ln(z) + \ln(1-z))(2\beta - \mathbb{H}_1 - \mathbb{H}_{-1}) \\
 & - 64z(3-z + \frac{z}{k^2})\ln(k)(\mathbb{H}_1 + \mathbb{H}_{-1}) + \frac{16(-1+z)\beta}{3z}(3-k^2-4z-4z^2)(6\ln(k) \\
 & - \ln(1-k^2) - 2\ln(k^2-z) - 2\mathbb{H}_0) - \frac{64z(k^2(z-3)-z)}{3k^2} \left[ \mathbb{H}_1\mathbb{H}_0 + \mathbb{H}_{-1,0} - \mathbb{H}_{0,1} \right. \\
 & \left. - \mathbb{H}_{1,w_4} - \mathbb{H}_{-1,w_4} - \mathbb{H}_{w_3,1} - \mathbb{H}_{w_3,-1} + \left( \frac{1}{2}\ln(1-k^2) + \ln(k^2-z) + \mathbb{H}_{w_3} \right) \right. \\
 & \left. \times (\mathbb{H}_1 + \mathbb{H}_{-1}) \right] - \frac{32z}{3k^2}(z+k^2(6-7z+3z^2))\ln(k^2-z^2)(\mathbb{H}_1 + \mathbb{H}_{-1}) \Big\} \\
 & + \frac{1}{2}P_{gq}^{(0)} \otimes \bar{h}_{L,g}^{(1)} \ln\left(\frac{Q^2}{\mu_F^2}\right) - P_{gq}^{(0)} \otimes \bar{b}_{L,g}^{(1)}, \tag{3.65}
 \end{aligned}$$

$$\begin{aligned}
 H_{1,q}^{(2),\text{PS}} &= C_{\text{FTF}} \left\{ -\frac{4(1-z)P_{28}}{k^2}(\mathbb{H}_{w_6,-1} - \mathbb{H}_{w_8,1} + \mathbb{H}_1\mathbb{H}_{w_8} - \mathbb{H}_{-1}\mathbb{H}_{w_6}) \right. \\
 & - \frac{8P_{29}}{3k^3}(\mathbb{H}_1\mathbb{H}_{w_1} - \mathbb{H}_{-1}\mathbb{H}_{w_2}) - \frac{8P_{30}}{3k^3}\mathbb{H}_1\mathbb{H}_{w_2} + \frac{8(k^2-z)P_{30}}{3k^5(1-z)\beta^2}\mathbb{H}_{w_1}\mathbb{H}_{-1} \\
 & + \frac{4(1-z)P_{31}}{k^2}(\mathbb{H}_{w_5,-1} - \mathbb{H}_{w_7,1} + \mathbb{H}_1\mathbb{H}_{w_7} - \mathbb{H}_{-1}\mathbb{H}_{w_5}) + \frac{8P_{32}}{3z} \left[ k(\mathbb{H}_{w_1}^2 - \mathbb{H}_{w_2}^2) \right. \\
 & + 2(\mathbb{H}_{w_1,w_4} + \mathbb{H}_{w_2,w_4} + \mathbb{H}_{w_3,w_1} + \mathbb{H}_{w_3,w_2}) + (\mathbb{H}_{w_1} + \mathbb{H}_{w_2})[6\ln(k) + \ln(k^2-z^2)] \\
 & + k(1-z)(\mathbb{H}_{w_5,w_1} + \mathbb{H}_{w_6,w_2} - \mathbb{H}_{w_7,w_2} - \mathbb{H}_{w_8,w_1} - \mathbb{H}_{w_1}\mathbb{H}_{w_5} - \mathbb{H}_{w_2}\mathbb{H}_{w_6} + \mathbb{H}_{w_2}\mathbb{H}_{w_7} \\
 & \left. + \mathbb{H}_{w_1}\mathbb{H}_{w_8}) - (\mathbb{H}_{w_1} + \mathbb{H}_{w_2})[\ln(1-k^2) + 2\ln(k^2-z) + 2\mathbb{H}_{w_3}] \right] \\
 & + \frac{16(1-z)\beta P_{33}}{9k^2z} + \frac{32P_{34}}{3k^4} \left[ \mathbb{H}_{0,1} - \mathbb{H}_{-1,0} - \mathbb{H}_0\mathbb{H}_1 + \mathbb{H}_{1,w_4} + \mathbb{H}_{w_3,1} + \mathbb{H}_{w_3,-1} + \mathbb{H}_{-1,w_4} \right. \\
 & \left. - (\mathbb{H}_1 + \mathbb{H}_{-1}) \left( \frac{1}{2}\ln(1-k^2) + \ln(k^2-z) + \mathbb{H}_{w_3} \right) \right] - \frac{32(1-z^2)P_{35}}{3k^2} \left[ \mathbb{H}_{w_9,1} \right. \\
 & \left. + \mathbb{H}_{w_9,-1} - (1-z)k(\mathbb{H}_{w_9,w_5} + \mathbb{H}_{w_9,w_6} + \mathbb{H}_{w_9,w_7} + \mathbb{H}_{w_9,w_8}) \right] + \frac{4(1-z)P_{36}}{3k^3}(\mathbb{H}_{w_5,1} \\
 & - \mathbb{H}_{w_7,-1} - \mathbb{H}_1\mathbb{H}_{w_5} + \mathbb{H}_{-1}\mathbb{H}_{w_7}) + \frac{4(1-z)P_{37}}{3k^3}(\mathbb{H}_{w_6,1} - \mathbb{H}_{w_8,-1} - \mathbb{H}_1\mathbb{H}_{w_6} + \mathbb{H}_{-1}\mathbb{H}_{w_8}) \\
 & + \frac{16P_{38}}{3k^4}(\mathbb{H}_{-1}\mathbb{H}_1 - 2\mathbb{H}_{-1,1}) - \frac{16(1-z)\beta P_{39}}{3k^2z}\ln(k^2-z^2) - \frac{8P_{40}}{3k^3z}(\mathbb{H}_{w_1,1} - \mathbb{H}_{w_2,-1})
 \end{aligned}$$

### 3. Unpolarized Pure-Singlet Wilson Coefficients at NLO

$$\begin{aligned}
& -\frac{8P_{41}}{3k^3z}H_{w_2,1} - \frac{16(1-z)\beta P_{42}}{3k^2z} \left[ \ln(1-k^2) + 2\ln(k^2-z) - 6\ln(k) + 2H_0 \right. \\
& \left. + 4H_{w_3} \right] - \frac{16P_{43}}{3k^2z}(H_{w_1,0} + H_{w_2,0}) - \frac{8P_{44}}{3k^4}(H_1^2 - H_{-1}^2) + \frac{16P_{45}}{3k^2z}(H_{w_1} + H_{w_2})H_0 \\
& + \frac{8(1-z)P_{45}}{3k^2z} \left[ H_{w_5,0} - H_{w_6,0} + H_{w_7,0} - H_{w_8,0} - (H_{w_5} - H_{w_6} + H_{w_7} - H_{w_8})H_0 \right] \\
& + \frac{4P_{46}}{3z^{3/2}k^3} \left[ 2H_{w_{10},w_1} + 2H_{w_{10},w_2} - (1-z) \left( H_{w_{10},w_5} - H_{w_{10},w_6} + H_{w_{10},w_7} - H_{w_{10},w_8} \right. \right. \\
& \left. \left. - k(H_{w_5,w_{11}} + H_{w_6,w_{11}} + H_{w_7,w_{11}} + H_{w_8,w_{11}}) + k(H_{w_5} + H_{w_6} + H_{w_7} + H_{w_8})H_{w_{11}} \right) \right. \\
& \left. + 2k(1-k^2)z(1-z) \left( H_{w_5,w_{12}} + H_{w_6,w_{12}} + H_{w_7,w_{12}} + H_{w_8,w_{12}} - (H_{w_5} + H_{w_6} + H_{w_7} \right. \right. \\
& \left. \left. + H_{w_8})H_{w_{12}} \right) + 2(1-k^2)z(H_{w_{12},1} + H_{w_{12},-1}) \right] + \frac{8P_{47}}{9k^2z(1+k\beta)}H_{w_2} \\
& - \frac{8P_{48}}{9k^2z(1-k\beta)}H_{w_1} - \frac{4(1-z)^2P_{49}}{3k^3z(k(z-2)-z)}H_{w_6} - \frac{4(1-z)^2P_{50}}{3k^3z(k(z-2)+z)}H_{w_5} \\
& - \frac{4(1-z)^2P_{51}}{3k^3z(k(z-2)+z)}H_{w_7} - \frac{4(1-z)^2P_{52}}{3k^3z(k(z-2)-z)}H_{w_8} - \frac{8P_{55}}{3k^5(1-z)z\beta^2}H_{w_1,-1} \\
& - \frac{8P_{53}}{9k^4z(1+\beta)(k^2(z-2)^2-z^2)}H_1 + \frac{8P_{54}}{9k^4z(1-\beta)(k^2(z-2)^2-z^2)}H_{-1} \\
& - \left[ \frac{16(1+k^2)(1-3k^2)z^2}{3k^4} \ln(k^2-z^2) + 16(1-z)(\ln(1-z) + \ln(z)) \right. \\
& \left. + 32 \left( 3(1-z) + \frac{(1+k^2)(1-3k^2)z^2}{k^4} \right) \ln(k) \right] (H_1 + H_{-1}) \\
& - 8 \frac{2k^2 + (3k^2-1)z}{k^2} \left[ 4H_{0,1,1} + 4H_{0,-1,1} - 20H_{1,1,1} - 4H_{1,1,w_4} - 4H_{1,-1,w_4} \right. \\
& + 4H_{w_3,1,1} - 4H_{w_3,1,-1} + 4H_{w_3,-1,1} - 4H_{w_3,-1,-1} - 4H_{-1,1,0} - 16H_{-1,1,1} + 4H_{-1,1,w_4} \\
& - 4H_{-1,-1,0} - 16H_{-1,-1,1} + 4H_{-1,-1,w_4} - 20H_{-1,-1,-1} + 2(H_1^2 - 2H_{-1,1})H_0 \\
& + 2(-4H_{-1,1} + H_1^2 - H_{-1}^2 + 2H_1H_{-1})H_{w_3} + (4H_{-1,1} - 5H_{-1}^2 + 5H_1^2 - 4H_{0,1} \\
& - 4H_{0,-1} - 4H_{w_3,1} - 4H_{w_3,-1})H_1 + (4H_0H_1 - H_1^2 + 4H_{w_3,1} + 4H_{w_3,-1} + 12H_{-1,1} \\
& + 5H_{-1}^2)H_{-1} - [\ln(1-k^2) - \ln(k^2-z^2) + 2\ln(k^2-z) - 6\ln(k)] \\
& \left. \times (4H_{-1,1} + H_{-1}^2 - H_1^2 - 2H_{-1}H_1) \right] - \frac{16(1-z)(z-k^2(2+3z))}{k} \left[ H_{1,w_4,w_5} \right. \\
& + H_{1,w_4,w_6} + H_{1,w_4,w_7} + H_{1,w_4,w_8} - H_{w_5,1,1} + H_{w_5,1,-1} - H_{w_5,w_3,1} + H_{w_5,w_3,-1} \\
& - H_{w_6,1,1} + H_{w_6,1,-1} - H_{w_6,w_3,1} + H_{w_6,w_3,-1} - H_{w_7,w_3,1} + H_{w_7,w_3,-1} + H_{w_7,-1,1} \\
& - H_{w_7,-1,-1} - H_{w_8,w_3,1} + H_{w_8,w_3,-1} + H_{w_8,-1,1} - H_{w_8,-1,-1} - H_{-1,w_4,w_5} - H_{-1,w_4,w_6} \\
& - H_{-1,w_4,w_7} - H_{-1,w_4,w_8} + k(H_{w_2,w_4,w_5} + H_{w_2,w_4,w_6} + H_{w_2,w_4,w_7} + H_{w_2,w_4,w_8} \\
& - H_{w_1,w_4,w_5} - H_{w_1,w_4,w_6} - H_{w_1,w_4,w_7} - H_{w_1,w_4,w_8} + H_{w_5,1,w_1} - H_{w_5,1,w_2} + H_{w_5,w_3,w_1} \\
& - H_{w_5,w_3,w_2} + H_{w_6,1,w_1} - H_{w_6,1,w_2} + H_{w_6,w_3,w_1} - H_{w_6,w_3,w_2} + H_{w_7,w_3,w_1} - H_{w_7,w_3,w_2} \\
& - H_{w_7,-1,w_1} + H_{w_7,-1,w_2} + H_{w_8,w_3,w_1} - H_{w_8,w_3,w_2} - H_{w_8,-1,w_1} + H_{w_8,-1,w_2}) \\
& + \{H_{w_3,1} - H_{w_3,-1} + H_{-1,1} + k[H_{w_1,1} - H_{w_2,1} - H_{w_3,w_1} + H_{w_3,w_2}]\} (H_{w_5} + H_{w_6}) \\
& + \{H_{w_3,1} - H_{w_3,-1} - H_{-1,1} - H_{-1,-1} + k[H_{w_2,-1} - H_{w_1,-1} - H_{w_3,w_1} + H_{w_3,w_2}]\} \\
& \times (H_{w_7} + H_{w_8}) + (H_{w_5,1} + H_{w_5,w_3} + H_{w_6,1} + H_{w_6,w_3} + H_{w_7,w_3} - H_{w_7,-1} + H_{w_8,w_3}
\end{aligned}$$

$$\begin{aligned}
 & -\mathbb{H}_{w_8,-1} - [\mathbb{H}_{w_5} + \mathbb{H}_{w_6} + \mathbb{H}_{w_7} + \mathbb{H}_{w_8}] \mathbb{H}_{w_3} (\mathbb{H}_1 - \mathbb{H}_{-1}) - k(\mathbb{H}_{w_5,1} + \mathbb{H}_{w_5,w_3} \\
 & + \mathbb{H}_{w_6,1} + \mathbb{H}_{w_6,w_3} + \mathbb{H}_{w_7,w_3} - \mathbb{H}_{w_7,-1} + \mathbb{H}_{w_8,w_3} - \mathbb{H}_{w_8,-1} - [\mathbb{H}_{w_5} + \mathbb{H}_{w_6} + \mathbb{H}_{w_7} \\
 & + \mathbb{H}_{w_8}] \mathbb{H}_{w_3} (\mathbb{H}_{w_1} - \mathbb{H}_{w_2}) + (\mathbb{H}_{w_7} + \mathbb{H}_{w_8}) \mathbb{H}_1 \mathbb{H}_{-1} - \frac{1}{2} (\mathbb{H}_{w_5} + \mathbb{H}_{w_6}) \mathbb{H}_1^2 \Big] \\
 & + 16(z - k^2(2 + 3z)) [\mathbb{H}_{w_1,1} + \mathbb{H}_{w_1,-1} - \mathbb{H}_{w_2,1} - \mathbb{H}_{w_2,-1}] (\mathbb{H}_{w_1} - \mathbb{H}_{w_2}) \\
 & + \frac{32(k^2(2 + 3z) - z)}{k} \Big[ \mathbb{H}_{w_1,1,0} + \mathbb{H}_{w_1,1,1} - \mathbb{H}_{w_1,1,w_4} - \mathbb{H}_{w_1,1,-1} + \mathbb{H}_{w_1,-1,0} + \mathbb{H}_{w_1,-1,1} \\
 & - \mathbb{H}_{w_1,-1,w_4} - \mathbb{H}_{w_1,-1,-1} - \mathbb{H}_{w_2,1,0} - \mathbb{H}_{w_2,1,1} + \mathbb{H}_{w_2,1,w_4} + \mathbb{H}_{w_2,1,-1} - \mathbb{H}_{w_2,-1,0} \\
 & - \mathbb{H}_{w_2,-1,1} + \mathbb{H}_{w_2,-1,w_4} + \mathbb{H}_{w_2,-1,-1} + \mathbb{H}_{w_3,1,w_1} - \mathbb{H}_{w_3,1,w_2} + \mathbb{H}_{w_3,-1,w_1} - \mathbb{H}_{w_3,-1,w_2} \\
 & + \frac{1}{2} [\mathbb{H}_{w_1,1} + \mathbb{H}_{w_1,-1} - \mathbb{H}_{w_2,1} - \mathbb{H}_{w_2,-1}] (2\mathbb{H}_{w_3} + \mathbb{H}_1 - \mathbb{H}_{-1}) + \frac{1}{4} [\mathbb{H}_1^2 - 4\mathbb{H}_{w_3,-1} \\
 & - 4\mathbb{H}_{w_3,1} - 4\mathbb{H}_{-1,1} - \mathbb{H}_{-1}^2 + 2\mathbb{H}_{-1}\mathbb{H}_1] (\mathbb{H}_{w_1} - \mathbb{H}_{w_2}) + \frac{1}{2} [\mathbb{H}_{w_2,-1} - \mathbb{H}_{w_1,1} - \mathbb{H}_{w_1,-1} \\
 & + \mathbb{H}_{w_2,1}] (6 \ln(k) - \ln(1 - k^2) + \ln(k^2 - z^2) - 2 \ln(k^2 - z)) \Big] \\
 & + 32(1 - z)\beta(\ln(1 - z) + \ln(z)) \Big\} + \frac{1}{2} P_{gq}^{(0)} \otimes \bar{h}_{1,g}^{(1)} \ln\left(\frac{Q^2}{\mu_F^2}\right) - P_{gq}^{(0)} \otimes \bar{b}_{1,g}^{(1)}, \quad (3.66)
 \end{aligned}$$

with the polynomials

$$P_1 = k^4 + k^2(2 - 6z) - 12z^2 + 6z - 3, \quad (3.67)$$

$$P_2 = -k^2 + 12z^3 - 16z^2 - 4z + 3, \quad (3.68)$$

$$P_3 = 8k^4 + k^2(-25z^2 - 28z + 12) + 9z^2, \quad (3.69)$$

$$P_4 = k^6 + k^4(3 - 6z^2) - 4z^4, \quad (3.70)$$

$$P_5 = k^2(z^2 - 3z - 1) - z^2 - 3z + 1, \quad (3.71)$$

$$P_6 = k^8 + k^6(-3z^2 - 3z + 2) - 3k^4(z^2 - z + 1) - 2k^2z^4 + 2z^4, \quad (3.72)$$

$$P_7 = 3k^6(z - 1) - 2k^5z(3z^2 - 7z + 6) + k^4(3 - 9z) - 2k^3z^2 + 2k^2z^3 - 2z^3, \quad (3.73)$$

$$P_8 = 3k^6(z - 1) + 2k^5z(3z^2 - 7z + 6) + k^4(3 - 9z) + 2k^3z^2 + 2k^2z^3 - 2z^3, \quad (3.74)$$

$$P_9 = k^4 + k^2(4z^2 + 3z - 3) + z(-4z^2 - 4z + 3), \quad (3.75)$$

$$P_{10} = k^2(5z^2 - 2) + 3z^2, \quad (3.76)$$

$$P_{11} = k^2(5z^2 - 15z + 1) - 5z^2 + 3z - 1, \quad (3.77)$$

$$P_{12} = k^4(-80z^3 + 35z^2 + 30z - 9) + 2k^2z(19z^2 - 10z - 9) + 3z^2(5z^2 + 2z + 1), \quad (3.78)$$

$$\begin{aligned}
 P_{13} &= 6k^5(z - 1) + k^4(-4z^3 + 21z^2 - 30z + 8) + k^3(4z^3 - 21z^2 + 12z - 2) + 3k^2z^2 \\
 &+ kz^2(4z - 3) - 4z^3, \quad (3.79)
 \end{aligned}$$

$$\begin{aligned}
 P_{14} &= 6k^5(z - 1) + k^4(4z^3 - 21z^2 + 30z - 8) + k^3(4z^3 - 21z^2 + 12z - 2) - 3k^2z^2 \\
 &+ kz^2(4z - 3) + 4z^3, \quad (3.80)
 \end{aligned}$$

$$\begin{aligned}
 P_{15} &= 3k^8 - 6k^6(z^2 + 2z - 1) + k^5z(12z^3 - 25z^2 + 6) - 3k^4(6z^2 - 4z + 3) - 2k^3z(z^2 \\
 &- 6z + 3) - 4k^2z^4 + 3kz^3 + 4z^4, \quad (3.81)
 \end{aligned}$$

$$\begin{aligned}
 P_{16} &= 6k^6(z - 1) + k^5(20z^3 - 35z^2 + 24z + 2) + k^4(6 - 18z) + 2k^3(2z^3 - 5z^2 + 6z - 1) \\
 &+ 4k^2z^3 - 3kz^2 - 4z^3, \quad (3.82)
 \end{aligned}$$

$$\begin{aligned}
 P_{17} &= -6k^6(z - 1) + k^5(20z^3 - 35z^2 + 24z + 2) + 6k^4(3z - 1) \\
 &+ 2k^3(2z^3 - 5z^2 + 6z - 1) - 4k^2z^3 - 3kz^2 + 4z^3, \quad (3.83)
 \end{aligned}$$

$$P_{18} = k^4(80z^3 - 35z^2 - 30z + 9) + 2k^2z(-19z^2 + 10z + 9) - 3z^2(5z^2 + 2z + 1), \quad (3.84)$$

$$P_{19} = 3k^8 - 6k^6(z^2 + 2z - 1) + k^5(-12z^4 + 25z^3 - 6z) - 3k^4(6z^2 - 4z + 3)$$

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$$+2k^3z(z^2 - 6z + 3) - 4k^2z^4 - 3kz^3 + 4z^4, \quad (3.85)$$

$$\begin{aligned} P_{20} = & 16\beta k^7 - 40k^6 + 8\beta k^5(18z^2 + 3z - 5) + 8k^4(36z^3 - 66z^2 - 15z + 17) \\ & + 3\beta k^3(192z^4 - 344z^3 + 69z^2 + 82z - 31) - 3k^2(192z^4 - 248z^3 - 59z^2 + 50z - 7) \\ & + 3\beta kz(25z^2 - 6z - 3) + 3z(-25z^2 + 6z + 3), \end{aligned} \quad (3.86)$$

$$\begin{aligned} P_{21} = & 16\beta k^7 + 40k^6 + 8\beta k^5(18z^2 + 3z - 5) - 8k^4(36z^3 - 66z^2 - 15z + 17) \\ & + 3\beta k^3(192z^4 - 344z^3 + 69z^2 + 82z - 31) + 3k^2(192z^4 - 248z^3 - 59z^2 + 50z - 7) \\ & + 3\beta kz(25z^2 - 6z - 3) + 3z(25z^2 - 6z - 3), \end{aligned} \quad (3.87)$$

$$\begin{aligned} P_{22} = & 8k^8(z-2)(\beta(z-1)+1) - 8k^7(-2\beta + \beta z^3 + (1-8\beta)z^2 + (9\beta-4)z + 2) \\ & + k^6(-66\beta + (68\beta - 96)z^4 + (328 - 186\beta)z^3 + (17\beta - 288)z^2 + (167\beta - 24)z + 48) \\ & + k^5(-30\beta - 192\beta z^5 + 4(207\beta - 41)z^4 + (314 - 935\beta)z^3 + 3(47\beta + 5)z^2 + \\ & (188\beta - 199)z + 66) + k^4(-192(\beta - 1)z^5 + 4(94\beta - 183)z^4 - 15(9\beta - 41)z^3 \\ & + (83 - 52\beta)z^2 + (3\beta - 100)z - 18) + k^3z(-6\beta + 192z^4 + 7(\beta - 40)z^3 + (7 - 18\beta)z^2 \\ & + (17\beta + 20)z + 21) + k^2(z-1)z((4\beta - 7)z^2 + (3\beta + 11)z - 6) \\ & - k(z-1)z^2((3\beta + 4)z + 3) + 3(z-1)z^3, \end{aligned} \quad (3.88)$$

$$\begin{aligned} P_{23} = & 72k^8(z-2)^2(\beta(z-1)+1) + k^6(108(8\beta-7) + 8(36\beta+29)z^5 - 2(576\beta+539)z^4 \\ & + (576\beta+1807)z^3 + 3(768\beta-563)z^2 - 1440(2\beta-1)z) + k^4z(-16(18\beta+17)z^4 \\ & + 208z^3 + (504\beta+95)z^2 - 3(72\beta+145)z + 360) + k^2z^2(43z^3 + 99z^2 - 150z + 36) \\ & - 3z^4(z+3), \end{aligned} \quad (3.89)$$

$$\begin{aligned} P_{24} = & 72k^8(z-2)^2(\beta(z-1)-1) + k^6(108(8\beta+7) + 8(36\beta-29)z^5 - 2(576\beta-539)z^4 \\ & + (576\beta-1807)z^3 + 3(768\beta+563)z^2 - 1440(2\beta+1)z) - k^4z(16(18\beta-17)z^4 \\ & + 208z^3 + (95-504\beta)z^2 + 3(72\beta-145)z + 360) - k^2z^2(43z^3 + 99z^2 - 150z + 36) \\ & + 3z^4(z+3), \end{aligned} \quad (3.90)$$

$$\begin{aligned} P_{25} = & 8k^8(z-2)(\beta(z-1)+1) + 8k^7(-2\beta + \beta z^3 + (1-8\beta)z^2 + (9\beta-4)z + 2) \\ & + k^6(-66\beta + (68\beta - 96)z^4 + (328 - 186\beta)z^3 + (17\beta - 288)z^2 + (167\beta - 24)z + 48) \\ & + k^5(30\beta + 192\beta z^5 + (164 - 828\beta)z^4 + (935\beta - 314)z^3 - 3(47\beta + 5)z^2 \\ & + (199 - 188\beta)z - 66) + k^4(-192(\beta - 1)z^5 + 4(94\beta - 183)z^4 - 15(9\beta - 41)z^3 \\ & + (83 - 52\beta)z^2 + (3\beta - 100)z - 18) - k^3z(-6\beta + 192z^4 + 7(\beta - 40)z^3 \\ & + (7 - 18\beta)z^2 + (17\beta + 20)z + 21) + k^2(z-1)z((4\beta - 7)z^2 + (3\beta + 11)z - 6) \\ & + k(z-1)z^2((3\beta + 4)z + 3) + 3(z-1)z^3, \end{aligned} \quad (3.91)$$

$$\begin{aligned} P_{26} = & -8k^8(z-2)(\beta(z-1)-1) + 8k^7(-2(\beta+1) + \beta z^3 - (8\beta+1)z^2 + (9\beta+4)z) \\ & - k^6(-6(11\beta+8) + (68\beta+96)z^4 - 2(93\beta+164)z^3 + (17\beta+288)z^2 + (167\beta+24)z) \\ & + k^5(30\beta + 192\beta z^5 - 4(207\beta+41)z^4 + (935\beta+314)z^3 - 3(47\beta-5)z^2 \\ & - (188\beta+199)z + 66) + k^4(192(\beta+1)z^5 - 4(94\beta+183)z^4 + 15(9\beta+41)z^3 \\ & + (52\beta+83)z^2 - (3\beta+100)z - 18) + k^3z(6\beta + 192z^4 - 7(\beta+40)z^3 \\ & + (18\beta+7)z^2 + (20-17\beta)z + 21) - k^2(z-1)z((4\beta+7)z^2 + (3\beta-11)z + 6) \\ & + k(z-1)z^2((3\beta-4)z-3) + 3(z-1)z^3, \end{aligned} \quad (3.92)$$

$$\begin{aligned} P_{27} = & 8k^8(z-2)(\beta(z-1)-1) + 8k^7(-2(\beta+1) + \beta z^3 - (8\beta+1)z^2 + (9\beta+4)z) \\ & + k^6(-6(11\beta+8) + (68\beta+96)z^4 - 2(93\beta+164)z^3 + (17\beta+288)z^2 + (167\beta+24)z) \\ & + k^5(30\beta + 192\beta z^5 - 4(207\beta+41)z^4 + (935\beta+314)z^3 - 3(47\beta-5)z^2 \\ & - (188\beta+199)z + 66) + k^4(-192(\beta+1)z^5 + 4(94\beta+183)z^4 - 15(9\beta+41)z^3 \\ & - (52\beta+83)z^2 + (3\beta+100)z + 18) + k^3z(6\beta + 192z^4 - 7(\beta+40)z^3 \end{aligned}$$

$$\begin{aligned}
& +(18\beta + 7)z^2 + (20 - 17\beta)z + 21) + k^2(z - 1)z((4\beta + 7)z^2 + (3\beta - 11)z + 6) \\
& + k(z - 1)z^2((3\beta - 4)z - 3) - 3(z - 1)z^3 \tag{3.93}
\end{aligned}$$

$$P_{28} = 3k^4(z - 2) + k^3(20 - 14z) + 6k^2(z + 1) + 2kz - z, \tag{3.94}$$

$$P_{29} = 9k^5(z - 2) - 6k^4z^2 + 18k^3(z + 1) - 4k^2z^2 - 3kz + 2z^2, \tag{3.95}$$

$$P_{30} = 9k^5(z - 2) + 6k^4z^2 + 18k^3(z + 1) + 4k^2z^2 - 3kz - 2z^2, \tag{3.96}$$

$$P_{31} = 3k^4(z - 2) + 2k^3(7z - 10) + 6k^2(z + 1) - 2kz - z, \tag{3.97}$$

$$P_{32} = 3k^4 - 2k^2(9z + 2) + 18z - 7, \tag{3.98}$$

$$P_{33} = 30k^4 + k^2(-60z^2 + 63z + 28) + 16z^2, \tag{3.99}$$

$$P_{34} = 3k^4(z^2 + z - 1) + 2k^2z^2 - z^2, \tag{3.100}$$

$$P_{35} = 3k^4(z^2 + 3) + k^2(2z^2 + 3) - z^2, \tag{3.101}$$

$$P_{36} = -9k^5(z - 2) + 6k^4(2z^2 - 7z + 10) - 18k^3(z + 1) + 2k^2z(4z + 3) + 3kz - 4z^2, \tag{3.102}$$

$$P_{37} = 9k^5(z - 2) + 6k^4(2z^2 - 7z + 10) + 18k^3(z + 1) + 2k^2z(4z + 3) - 3kz - 4z^2, \tag{3.103}$$

$$P_{38} = 3k^4(z - 8)z + k^2(2z^2 + 9z - 3) - z^2, \tag{3.104}$$

$$P_{39} = 3k^4 - k^2(6z^2 + 7) + 2z^2, \tag{3.105}$$

$$\begin{aligned}
P_{40} = & 9k^7 - 3k^5(3z^2 + 12z + 4) - 6k^4z^2(2z + 11) - 3k^3(6z^2 - 12z + 7) \\
& - 2k^2z(4z^2 - 9z + 6) + 3kz^2 + 4z^3, \tag{3.106}
\end{aligned}$$

$$\begin{aligned}
P_{41} = & 9k^7 - 3k^5(3z^2 + 12z + 4) + 6k^4z^2(2z + 11) - 3k^3(6z^2 - 12z + 7) \\
& + 2k^2z(4z^2 - 9z + 6) + 3kz^2 - 4z^3, \tag{3.107}
\end{aligned}$$

$$P_{42} = -3k^4 + k^2(6z^2 + 6z + 7) - 2z^2, \tag{3.108}$$

$$P_{43} = 6k^6 - k^4(9z^2 + 18z + 8) - 2k^2(9z^2 - 9z + 7) + 3z^2, \tag{3.109}$$

$$P_{44} = 3k^4(5z^2 + 14z - 6) + k^2(10z^2 - 9z + 3) - 5z^2, \tag{3.110}$$

$$P_{45} = 3k^6 - k^4(9z^2 + 4) - k^2(18z^2 + 7) + 3z^2, \tag{3.111}$$

$$P_{46} = 3k^4(6z^3 + 9z^2 - z + 2) + k^2z(3z^2 + 8z + 9) - z^2(3z + 1), \tag{3.112}$$

$$\begin{aligned}
P_{47} = & 6\beta k^7 + 24k^6 + 2\beta k^5(27z^2 + 27z + 28) + 2k^4(9z^2 + 27z - 2) \\
& - \beta k^3(36z^3 + 27z^2 - 93z + 52) + k^2(-36z^3 + 21z^2 + 93z - 10) \\
& + 3\beta kz(4z^2 + z - 1) + 3z(4z^2 - 3z - 1), \tag{3.113}
\end{aligned}$$

$$\begin{aligned}
P_{48} = & 6\beta k^7 - 24k^6 + 2\beta k^5(27z^2 + 27z + 28) - 2k^4(9z^2 + 27z - 2) \\
& - \beta k^3(36z^3 + 27z^2 - 93z + 52) + k^2(36z^3 - 21z^2 - 93z + 10) \\
& + 3\beta kz(4z^2 + z - 1) + 3z(-4z^2 + 3z + 1), \tag{3.114}
\end{aligned}$$

$$\begin{aligned}
P_{49} = & -6(\beta - 1)k^7(z - 2) + 6k^6z(\beta + z - 6) + k^5(-28\beta + 3(4\beta - 3)z^3 - 3(8\beta - 5)z^2 \\
& + 2(7\beta - 22)z + 40) + k^4((9 - 12\beta)z^3 - 8z^2 + (30 - 14\beta)z + 12) \\
& + 2k^3z(-2\beta z^2 + (4\beta + 2)z + 7) + 2k^2z(2\beta z^2 + z - 1) + k(z - 3)z^2 - z^3, \tag{3.115}
\end{aligned}$$

$$\begin{aligned}
P_{50} = & -6(\beta - 1)k^7(z - 2) - 6k^6z(\beta + z - 6) + k^5(-28\beta + 3(4\beta - 3)z^3 - 3(8\beta - 5)z^2 \\
& + 2(7\beta - 22)z + 40) + k^4(3(4\beta - 3)z^3 + 8z^2 + 2(7\beta - 15)z - 12) \\
& + 2k^3z(-2\beta z^2 + (4\beta + 2)z + 7) - 2k^2z(2\beta z^2 + z - 1) + k(z - 3)z^2 + z^3, \tag{3.116}
\end{aligned}$$

$$\begin{aligned}
P_{51} = & 6(\beta + 1)k^7(z - 2) - 6k^6z(-\beta + z - 6) + k^5(28\beta - 3(4\beta + 3)z^3 + 3(8\beta + 5)z^2 \\
& - 2(7\beta + 22)z + 40) - k^4(3(4\beta + 3)z^3 - 8z^2 + 2(7\beta + 15)z + 12) \\
& + 2k^3z(2\beta z^2 + (2 - 4\beta)z + 7) + 2k^2z(2\beta z^2 - z + 1) + k(z - 3)z^2 + z^3, \tag{3.117}
\end{aligned}$$

$$\begin{aligned}
P_{52} = & 6(\beta + 1)k^7(z - 2) + 6k^6z(-\beta + z - 6) + k^5(28\beta - 3(4\beta + 3)z^3 + 3(8\beta + 5)z^2 \\
& - 2(7\beta + 22)z + 40) + k^4(3(4\beta + 3)z^3 - 8z^2 + 2(7\beta + 15)z + 12) \\
& + 2k^3z(2\beta z^2 + (2 - 4\beta)z + 7) - 2k^2z(2\beta z^2 - z + 1) + k(z - 3)z^2 - z^3, \tag{3.118}
\end{aligned}$$

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$$\begin{aligned}
P_{53} &= 54\beta k^8(z-2)^2 z - 3k^6(-24(\beta+1) + (\beta-35)z^5 + (5\beta+113)z^4 - (47\beta+125)z^3 \\
&\quad + 6(15\beta+31)z^2 - 240z) + k^4 z(72(3\beta-4) + (59\beta-193)z^4 + (187-173\beta)z^3 \\
&\quad + 2(82\beta-143)z^2 - 6(17\beta+5)z) - k^2 z^2(12(\beta+1) + 3(23\beta-37)z^3 \\
&\quad + (11-25\beta)z^2 + (103\beta-167)z) + z^4(3\beta+13\beta z - 23z+3), \tag{3.119}
\end{aligned}$$

$$\begin{aligned}
P_{54} &= 54\beta k^8(z-2)^2 z - 3k^6(-24(\beta-1) + (\beta+35)z^5 + (5\beta-113)z^4 + (125-47\beta)z^3 \\
&\quad + 6(15\beta-31)z^2 + 240z) + k^4 z(72(3\beta+4) + (59\beta+193)z^4 - (173\beta+187)z^3 \\
&\quad + 2(82\beta+143)z^2 - 6(17\beta-5)z) - k^2 z^2(12(\beta-1) + 3(23\beta+37)z^3 \\
&\quad - (25\beta+11)z^2 + (103\beta+167)z) + z^4(3\beta+13\beta z + 23z-3), \tag{3.120}
\end{aligned}$$

$$\begin{aligned}
P_{55} &= 9\beta^2 k^9(z-1) + k^7(12\beta^2 + (9-54\beta^2)z^2 + 6(7\beta^2-3)z) + 6k^6 z^2(-11\beta^2 \\
&\quad + 3\beta^2 z^2 + 8\beta^2 z + z) + k^5(21\beta^2 - 9z^3 + 18(3\beta^2+2)z^2 + (18-75\beta^2)z) \\
&\quad + 2k^4 z(-6\beta^2 + (6\beta^2-3)z^3 + (2-15\beta^2)z^2 + 15\beta^2 z) \\
&\quad - 3k^3 z^2(6z+7) - 2k^2 z^3(-3\beta^2 + (3\beta^2+2)z+1) + 3kz^3 + 2z^4. \tag{3.121}
\end{aligned}$$

The remaining Mellin convolutions in Eqs. (3.65,3.66) are given in Appendix D.4. The Wilson coefficient  $H_{2,q}^{(2),\text{PS}}$  is given by

$$H_{2,q}^{(2),\text{PS}} = \frac{1}{2} \left( H_{1,q}^{(2),\text{PS}} + 3H_{L,q}^{(2),\text{PS}} \right). \tag{3.122}$$

In summary, the two-loop massive Wilson coefficients are represented in terms of iterated integrals over the alphabets given in Section 3.3. The integrals can be arranged such that only the last integral contains elliptic letters and all other integrals can be expressed in terms of classical polylogarithms with involved arguments. Some details are discussed in Appendix D.5. Similar structures are expected also for other physical processes depending on two scales,  $z$  and  $m^2/Q^2$ , in a non-factorizing manner. Even more involved structures will emerge in the case of more scales. The two-loop heavy flavor contributions to the structure functions  $F_{2(L)}$  are given by

$$F_{2(L)}^{(2),\text{PS, heavy}}(x, Q^2) = a_s^2(Q^2) Q_H^2 x H_{2(L)}^{\text{PS},(2)} \left( \frac{Q^2}{\mu^2}, x \right) \otimes \Sigma(x, \mu^2). \tag{3.123}$$

### 3.5. The asymptotic and threshold expansions

The complete expressions calculated in Section 3.4 allow now to perform the asymptotic expansion for  $Q^2 \gg m^2$  and the threshold expansion for  $\beta \ll 1$ . In the asymptotic limit  $Q^2 \gg m^2$  the massive pure singlet Wilson coefficient have the following representations [179, 185]

$$H_{L,q}^{(2),\text{PS}} \left( z, \frac{Q^2}{m^2} \right) = \tilde{C}_{q,L}^{(2),\text{PS}}(N_F+1), \tag{3.124}$$

$$H_{2,q}^{(2),\text{PS}} \left( z, \frac{Q^2}{m^2} \right) = A_{Qq}^{(2),\text{PS}}(N_F+1) + \tilde{C}_{q,2}^{(2),\text{PS}}(N_F+1). \tag{3.125}$$

Here the massless Wilson coefficients  $\tilde{C}_{q,L}^{(2),\text{PS}}(N_F+1)$  are the ones given in Section 3.2 normalized by  $N_F+1$ . The massive two-loop operator matrix element  $A_{Qq}^{(2),\text{PS}}$  in Mellin space in the  $\overline{\text{MS}}$  scheme [179, 185] reads

$$A_{Qq}^{(2),\text{PS}} = -\frac{1}{8} \hat{P}_{qg}^{(0)} P_{gq}^{(0)} \ln^2 \left( \frac{m^2}{\mu^2} \right) - \frac{1}{2} \hat{P}_{qg}^{(1),\text{PS}} \ln \left( \frac{m^2}{\mu^2} \right) + \frac{1}{8} \hat{P}_{qg}^{(0)} P_{gq}^{(0)} \zeta_2 + a_{Qq}^{(2),\text{PS}}. \tag{3.126}$$



The constant part of the unrenormalized OME  $a_{Qq}^{(2),\text{PS}}$  is given by

$$\begin{aligned}
 a_{Qq}^{(2),\text{PS}}(z) = & C_F T_F \left\{ -\frac{4(1-z)(112+121z+400z^2)}{27z} - \left( \frac{8}{9}(21+33z+56z^2) + 8(1+z)\zeta_2 \right) H_0 \right. \\
 & + \frac{2}{3}(3+15z+8z^2)H_0^2 - \frac{4}{3}(1+z)H_0^3 + \frac{8(1-z)(4+7z+4z^2)}{3z} H_0 H_1 \\
 & - \left[ \frac{8(1-z)(4+7z+4z^2)}{3z} - 16(1+z)H_0 \right] H_{0,1} \\
 & \left. - 32(1+z)H_{0,0,1} - \frac{4(1-z)(4+7z+4z^2)}{3z} \zeta_2 + 32(1+z)\zeta_3 \right\} \quad (3.127)
 \end{aligned}$$

in  $z$ -space.

Expanding the fully massive result given in Section 3.4 in the asymptotic limit  $Q^2 \gg m^2$  and setting  $\mu^2 = Q^2$  we find

$$\begin{aligned}
 H_{L,q}^{(2),\text{PS}} = & -32C_F T_F \left\{ \frac{(1-z)(1-2z+10z^2)}{9z} - (1+z)(1-2z)H_0 - zH_0^2 \right. \\
 & + \frac{(1-z)(1-2z-2z^2)}{3z} H_1 - zH_{0,1} + z\zeta_2 + \frac{m^2}{Q^2} \left[ -\frac{(1-z)(2-z+2z^2)}{3z} \ln^2 \left( \frac{m^2}{Q^2} \right) \right. \\
 & + \frac{(1-z)(-22+4z+29z^2)}{9z} - \left( \frac{(1-z)(20-7z-25z^2)}{9z} + \frac{2}{3}(3-6z \right. \\
 & \left. \left. - 2z^2)H_0 \right) \ln \left( \frac{m^2}{Q^2} \right) + \left( \frac{2}{9}(-6+3z+13z^2) + \frac{2(1+z)(-2+z+2z^2+2z^3)}{3z} \right. \right. \\
 & \left. \left. \times H_{-1} \right) H_0 - \frac{2}{3}z^3 H_0^2 + \left( -\frac{(1-z)^2(14+13z)}{9z} + \frac{4(1-z)(2-z+2z^2)}{3z} H_0 \right) H_1 \right. \\
 & + \frac{(1-z)(2-z+2z^2)}{3z} H_1^2 - \frac{2(4-3z-4z^3)}{3z} H_{0,1} \\
 & \left. + \frac{2(1+z)(2-z-2z^2-2z^3)}{3z} H_{0,-1} - \frac{2(1-z)(2-z+2z^2+2z^3)}{3z} \zeta_2 \right] \\
 & + \left( \frac{m^2}{Q^2} \right)^2 \left[ \frac{1}{2z}(4-2z-z^2-2z^3+4z^4) \ln^2 \left( \frac{m^2}{Q^2} \right) + \left( 2(2-3z+4z^3)H_0 \right. \right. \\
 & + \frac{(1-z)(28-20z+13z^2+21z^3)}{6z} + (2-3z-2z^2+4z^3)H_1 \left. \right) \ln \left( \frac{m^2}{Q^2} \right) \\
 & + \frac{1}{1152z}(16027-13011z-6267z^2+7571z^3+4320z^4) + \left( \frac{1}{3}(24-21z+16z^2 \right. \\
 & \left. - 21z^3) + \frac{4(1-z^2+z^3+2z^4)}{z} H_{-1} \right) H_0 - \left( \frac{1}{6z}(4-15z^2-16z^3+21z^4) \right. \\
 & \left. + \frac{4(2-2z+z^2)}{z} H_0 \right) H_1 - \frac{1}{2z}(4-6z+5z^2+2z^3-4z^4) H_1^2 \\
 & + \frac{2(4-2z-z^2+4z^4)}{z} H_{0,1} - \frac{4(1-z^2+z^3+2z^4)}{z} H_{0,-1} \\
 & \left. + \frac{2(2-2z+z^2)}{z} \zeta_2 \right] \left. \right\} + \mathcal{O}(\kappa^3 \ln^2(\kappa)) \quad , \quad (3.128)
 \end{aligned}$$

### 3. Unpolarized Pure-Singlet Wilson Coefficients at NLO

$$\begin{aligned}
H_{(2),q}^{2,\text{PS}} = & C_F T_F \left\{ - \left( \frac{4(1-z)(4+7z+4z^2)}{3z} + 8(1+z)H_0 \right) \ln^2 \left( \frac{m^2}{Q^2} \right) \right. \\
& - \left( \frac{16(1-z)(10+z+28z^2)}{9z} + \frac{8}{3}(3+15z+8z^2)H_0 \right. \\
& \left. \left. - 8(1+z)H_0^2 \right) \ln \left( \frac{m^2}{Q^2} \right) + \frac{16(1-z)(5+24z-52z^2)}{9z} \right. \\
& + \left( \frac{8}{9}(105-99z-88z^2) - \frac{32(1+z)^3}{3z}H_{-1} \right) H_0 + 8z(5-2z)H_0^2 + \frac{16}{3}(1+z)H_0^3 \\
& - \left( \frac{16(1-z)(13-26z+4z^2)}{9z} - \frac{16(1-z)(4+7z+4z^2)}{3z}H_0 \right) H_1 \\
& + \frac{4(1-z)(4+7z+4z^2)}{3z}H_1^2 + \left( -\frac{16(4+3z-3z^2+2z^3)}{3z} + 32(1+z)H_0 \right) H_{0,1} \\
& + \frac{32(1+z)^3}{3z}H_{0,-1} - 32(1+z)H_{0,0,1} + 16(1+z)H_{0,1,1} - \left( \frac{32(1+3z^2-3z^3)}{3z} \right. \\
& \left. + 32(1+z)H_0 \right) \zeta_2 + 16(1+z)\zeta_3 + \frac{m^2}{Q^2} \left[ \left( \frac{16(1-z)(1+2z^2)}{z} + 16zH_0 \right) \ln^2 \left( \frac{m^2}{Q^2} \right) \right. \\
& + \left( \frac{64(1-z)(2-z-4z^2)}{3z} + 32(1-3z-2z^2)H_0 - 16zH_0^2 \right) \ln \left( \frac{m^2}{Q^2} \right) \\
& + \frac{8(76-24z-102z^2+59z^3)}{9z} + \left( \frac{32(1+z)(1-z-2z^2-2z^3)}{z} H_{-1} \right. \\
& + \frac{16}{3}(6+27z-20z^2) \left. \right) H_0 + 32z(1+z^2)H_0^2 - \frac{32}{3}zH_0^3 - \frac{16(1-z)(1+2z^2)}{z}H_1^2 \\
& + \left( \frac{16(4-6z-9z^2+8z^3)}{3z} - \frac{64(1-z)(1+2z^2)}{z}H_0 \right) H_1 \\
& + \left( \frac{32(2-z+z^2-4z^3)}{z} - 64zH_0 \right) H_{0,1} - \frac{32(1+z)(1-z-2z^2-2z^3)}{z}H_{0,-1} \\
& + 64zH_{0,0,1} - 32zH_{0,1,1} + \left( \frac{32(1+z)(1-2z+2z^2-2z^3)}{z} + 64zH_0 \right) \zeta_2 - 32z\zeta_3 \left. \right] \\
& + \left( \frac{m^2}{Q^2} \right)^2 \left[ -\frac{4P_{61}}{3z} \ln^2 \left( \frac{m^2}{Q^2} \right) - \left( \frac{4P_{65}}{9(1-z)z} + \frac{16}{3}(9-33z-16z^2+72z^3)H_0 \right. \right. \\
& + 8(3-11z-12z^2+24z^3)H_1 \left. \right) \ln \left( \frac{m^2}{Q^2} \right) + \frac{64P_{59}}{3z}H_{0,-1} - \frac{4P_{60}}{3z}H_1^2 - \frac{16P_{62}}{3z}H_{0,1} \\
& - \frac{P_{66}}{72(1-z)^2z} - \left( \frac{64P_{59}}{3z}H_{-1} + \frac{16P_{63}}{9(1-z)} \right) H_0 + 64z^2H_0^2 - \left( \frac{4P_{64}}{9(1-z)z} \right. \\
& \left. \left. - \frac{32(16-9z-3z^2+8z^3)}{3z}H_0 \right) H_1 - \frac{16(16-9z-3z^2+24z^3)}{3z}\zeta_2 \right] \left. \right\} \\
& + \mathcal{O}(\kappa^3 \ln^2(\kappa)) , \tag{3.129}
\end{aligned}$$

with the polynomials

$$P_{59} = 18z^4 + 7z^3 - 9z^2 + 4 , \tag{3.130}$$

$$P_{60} = 72z^4 - 52z^3 - 27z^2 + 27z - 32 , \tag{3.131}$$

$$P_{61} = 72z^4 - 20z^3 - 39z^2 - 9z + 32 , \tag{3.132}$$

$$P_{62} = 72z^4 - 8z^3 - 39z^2 - 9z + 32, \quad (3.133)$$

$$P_{63} = 180z^4 - 391z^3 + 265z^2 - 111z + 66, \quad (3.134)$$

$$P_{64} = 360z^5 - 898z^4 + 667z^3 - 132z^2 + 118z - 88, \quad (3.135)$$

$$P_{65} = 360z^5 - 826z^4 + 529z^3 + 180z^2 - 362z + 128, \quad (3.136)$$

$$P_{66} = 12816z^6 - 6615z^5 - 51371z^4 + 62178z^3 + 7650z^2 - 43867z + 17673. \quad (3.137)$$

We note that the asymptotic terms are exactly reproduced, cf. [179, 185, 254], proving the asymptotic factorization in this process. The additional power suppressed terms can be used to obtain fast numerical implementations for the heavy quark Wilson coefficients which are valid for lower values of  $Q^2$ . The reach of this approximations is discussed in Section 3.6.

The threshold expansion of the Wilson coefficients for  $\beta \ll 1$  is given by

$$H_{L,g}^{(1)}\left(z, \frac{Q^2}{m^2}\right) = 32T_F z(1-z)\beta^3 \left\{ \frac{1}{3} + \frac{\beta^2}{15} + \frac{\beta^4}{35} + \frac{\beta^6}{63} \right\} + \mathcal{O}(\beta^{11}), \quad (3.138)$$

$$H_{2,g}^{(1)}\left(z, \frac{Q^2}{m^2}\right) = 4T_F \beta \left\{ 1 + \frac{2}{3}(3-2z)\beta^2 - \frac{2}{15}(3-10z+4z^2)\beta^4 + \frac{2}{105}(5+2z+8z^2)\beta^6 + \frac{2}{315}(21-22z+36z^2)\beta^8 \right\} + \mathcal{O}(\beta^{11}), \quad (3.139)$$

$$H_{L,q}^{(2),\text{PS}}\left(z, \frac{Q^2}{m^2}\right) = C_F T_F z(1-z)^2 \beta^5 \left[ -\frac{9856}{225} + \frac{128}{15} [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] - \beta^2 \left( \frac{256}{11025} (2785 - 2186z) - \frac{256}{105} (5-4z) [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] \right) - \beta^4 \left( \frac{256}{297675} (93721 - 162830z + 73888z^2) - \frac{128}{945} (121 - 200z + 88z^2) [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] \right) \right] + \mathcal{O}(\beta^{11}), \quad (3.140)$$

$$H_{2,q}^{(2),\text{PS}}\left(z, \frac{Q^2}{m^2}\right) = C_F T_F (1-z)\beta^3 \left[ -\frac{208}{9} + \frac{16}{3} [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] - \beta^2 \left( \frac{16}{225} (817 - 496z) - \frac{16}{15} (11 - 8z) [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] \right) - \beta^4 \left( \frac{64}{11025} (10649 - 11942z + 2358z^2 + 1260z^3) - \frac{16}{105} (79 - 112z + 48z^2) [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] \right) - \beta^6 \left( \frac{32}{297675} (673297 - 1361520z + 934476z^2 - 13048z^3 - 120960z^4) - \frac{16}{945} (817 - 1800z + 1536z^2 - 448z^3) [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] \right) \right] + \mathcal{O}(\beta^{11}). \quad (3.141)$$

### 3.6. Numerical results

Let us now illustrate the analytic results numerically. In Fig. 3.2 the two-loop heavy flavor Wilson coefficients are illustrated as a function of  $z$  for different values of  $Q^2 \in [10, 10^4] \text{ GeV}^2$ , setting the charm quark mass to  $m_c = 1.59 \text{ GeV}$ , cf. [256]. For large values of  $Q^2$  these results compare to Ref. [257] for  $H_{2,q}^{(2),\text{PS}}$ .

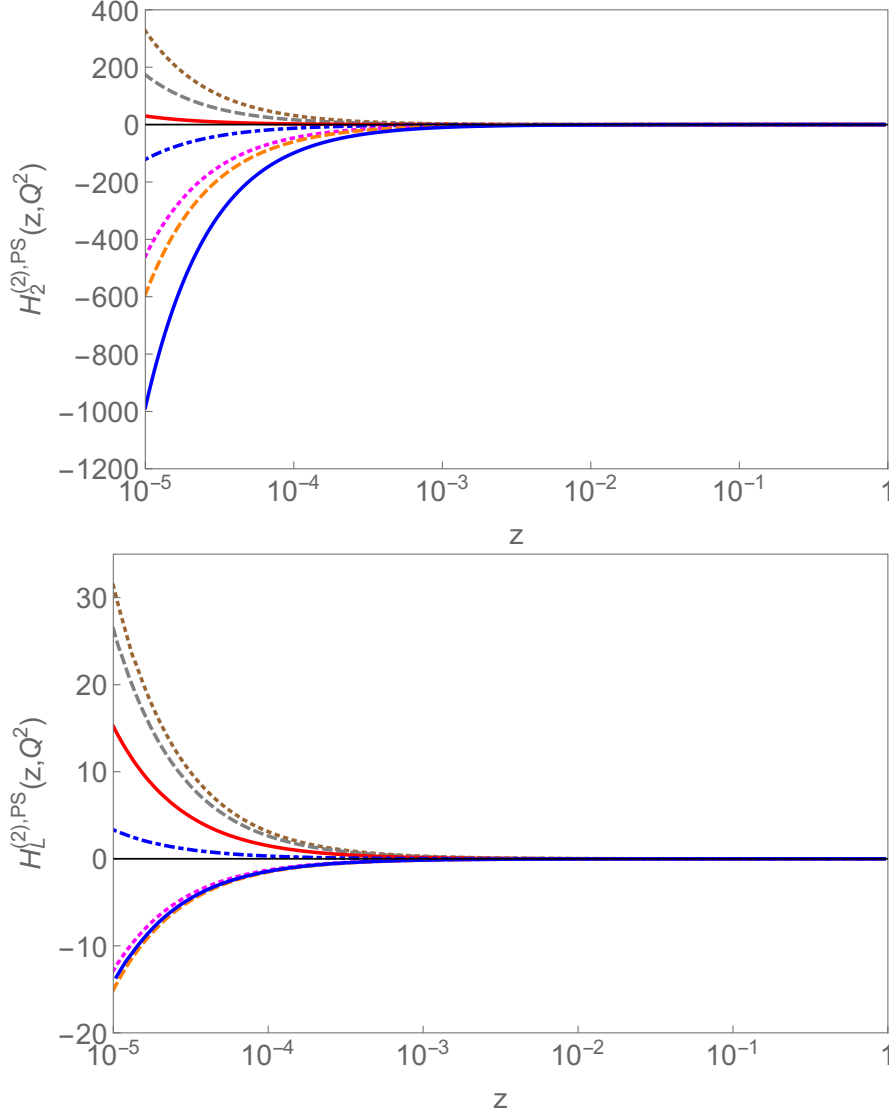


Figure 3.2.: The Wilson coefficients  $H_{2,q}^{(2),\text{PS}}$  (upper panel) and  $H_{L,q}^{(2),\text{PS}}$  (lower panel) as a function of  $z$  for different values of  $Q^2$  and the scale choice  $\mu^2 = \mu_F^2 = Q^2$ . Lower full line (Blue):  $Q^2 = 10^4 \text{ GeV}^2$ ; lower dashed line (Orange):  $Q^2 = 10^3 \text{ GeV}^2$ ; lower dotted line (Magenta):  $Q^2 = 500 \text{ GeV}^2$ ; dash-dotted line (Blue):  $Q^2 = 100 \text{ GeV}^2$ ; upper full line (Red):  $Q^2 = 50 \text{ GeV}^2$ ; upper dashed line (Gray):  $Q^2 = 25 \text{ GeV}^2$ ; upper dotted line (Brown):  $Q^2 = 10 \text{ GeV}^2$ .

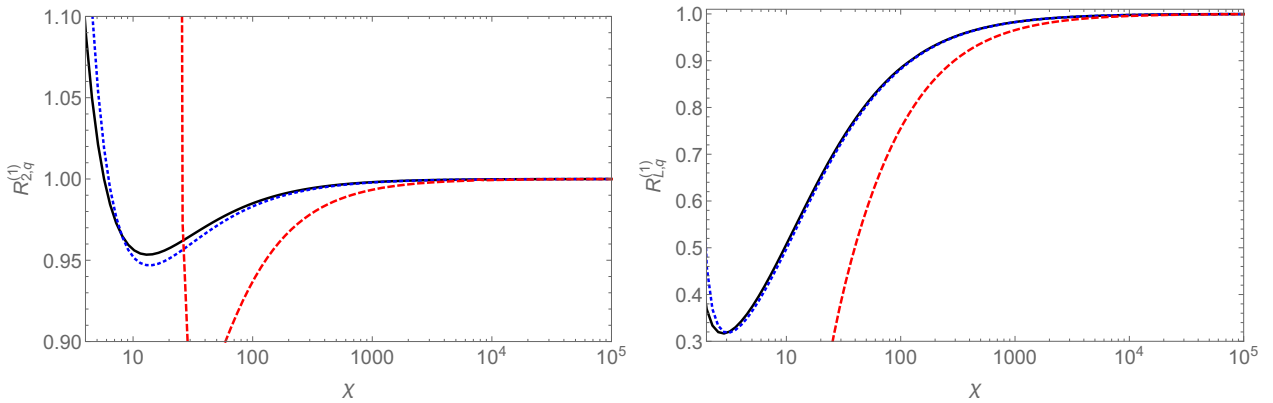


Figure 3.3.: The ratios  $R_{2,q}^{(1)}$  (left) and  $R_{L,q}^{(1)}$  (right), Eq. (3.142), as a function of  $\chi = Q^2/m^2$ . Solid line:  $z = 10^{-4}$ ; dotted line:  $z = 10^{-2}$ ; dashed line:  $z = 1/2$ .

Next we study the ratios

$$R_{i,q}^{(1)} = \frac{H_{i,q}^{(2),\text{PS}}}{\tilde{H}_{i,q}^{(2),\text{PS}}}(\mu = \mu_F = m), \quad (3.142)$$

cf. also [179], comparing the full, cf. Eqs. (3.65, 3.122) and the asymptotic results,  $\tilde{H}$ , cf. Eqs. (3.124, 3.125) in Fig. 3.3. For  $H_{2,q}^{(2),\text{PS}}$  the asymptotic expansion agrees with the full calculation up to  $Q^2/m^2 \equiv \chi = 100$  to about 2% for the small values of  $z = 10^{-4}, 10^{-2}$ . Extending the asymptotic representation down to  $\chi = 10$  does not introduce an error larger than 5% in this region. At larger  $z$  (here  $z = 1/2$ ) the asymptotic representation begins to deviate significantly from the full calculation beginning at  $\chi \sim 1000$ . However, the Wilson coefficients are very small in this region. As it was already noted earlier [179] the asymptotic representation for  $H_{L,q}^{(2),\text{PS}}$  is only valid for much higher values of  $\chi$ . Demanding an agreement of  $\leq 2\%$  requires  $\chi > 900$  for the small values of  $z$  and even higher values for larger  $z$ . Similar to the ratio of the full and asymptotic Wilson coefficient we define the ratio

$$R_{F_i} = \frac{F_{i,q}^{(2),\text{PS}}}{\tilde{F}_{i,q}^{(2),\text{PS}}}, \quad (3.143)$$

where  $\tilde{F}_{i,q}^{(2),\text{PS}}$  is the structure function obtained by using the expansion of the respective Wilson coefficient up the desired level. The corresponding results are depicted in Fig. 3.4. We use the parameterization of the parton distribution [207] at NNLO to better compare previous numerical results [257]. We used the LHAPDF interface [298]. Demanding an agreement within  $\pm 2\%$  for  $F_2$  in the range  $z \in [10^{-4}, 10^{-2}, 1/2]$  leads to values  $Q_0^2/m^2 \in [8, 9, 15]$  of the  $\mathcal{O}((m^2/Q^2)^2)$  improved result,  $Q_0^2/m^2 \in [10, 12, 30]$  of the  $\mathcal{O}(m^2/Q^2)$  improved result, and  $Q_0^2/m^2 \in [70, 80, 300]$  for the asymptotic result. For  $F_L$  the corresponding values are  $Q_0^2/m^2 \in [15, 15, 30]$  of the  $\mathcal{O}((m^2/Q^2)^2)$  improved result,  $Q_0^2/m^2 \in [15, 18, 40]$  of the  $\mathcal{O}(m^2/Q^2)$  improved result, and  $Q_0^2/m^2 \in [200, 200, 700]$  for the asymptotic result. The values of  $Q_0^2$  for  $F_L$  are thus larger than those for  $F_2$ .

In Figures 3.5 we show the complete results for the two-loop pure singlet contributions to  $F_2$  and  $F_L$  as a function of  $x$  for a series of  $Q^2$ -values. At large values of  $Q^2$  the corrections are negative and turn to positive values around  $Q^2 \sim 10 \text{ GeV}^2$ . In the small  $x$  region the corrections are large and grow with  $Q^2$ . The absolute corrections to  $F_L$  are smaller in size than those to  $F_2$ .

In Fig. 3.6 we illustrate the ratios Eq. (3.143) as a function of  $x$  for different values of  $Q^2$  for  $F_2$  and  $F_L$  comparing the asymptotic result to the full result. The corrections behave widely flat in  $x$ ,

### 3. Unpolarized Pure-Singlet Wilson Coefficients at NLO

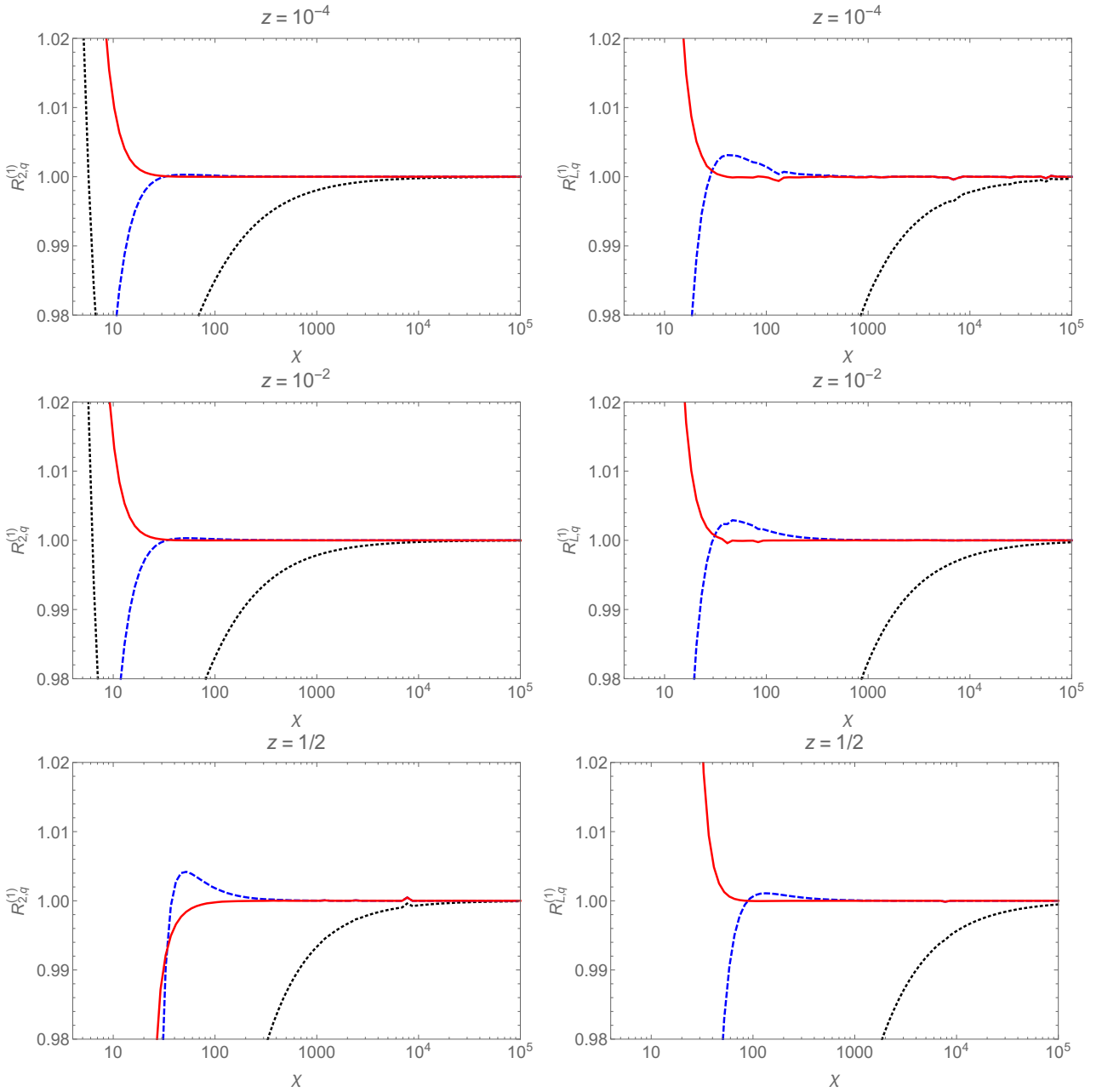


Figure 3.4.: The ratios  $R_{2,q}^{(1)}$  (left) and  $R_{L,q}^{(1)}$  (right), Eq. (3.142), as a function of  $\chi = Q^2/m^2$  for different values of  $z$  gradually improved with  $\kappa$  suppressed terms. Dotted lines: asymptotic result; dashed lines:  $\mathcal{O}(m^2/Q^2)$  improved; solid lines :  $\mathcal{O}((m^2/Q^2)^2)$  improved.

turning to lower values in the large  $x$  region. For  $F_2$  the ratios are larger than 0.96 for  $Q^2 \geq 500 \text{ GeV}^2$ . At  $Q^2 = 100 \text{ GeV}^2$ , values of  $\sim 0.85$  are obtained. For lower values of  $Q^2$  the ratio is even smaller.

For  $F_L$  the corrections are generally larger. At  $Q^2 = 10^4 \text{ GeV}^2$  one obtains a ratio of 0.96, for  $Q^2 = 10^3 \text{ GeV}^2$  0.85, and for  $Q^2 = 500 \text{ GeV}^2 \sim 0.75$ , with even larger deviations from one for lower values of  $Q^2$ .

In Fig. 3.7 we depict the ratio of the full result over the  $\mathcal{O}((m^2/Q^2)^2)$  improved asymptotic results for  $F_2$  and  $F_L$  as a function of  $x$  for a series of  $Q^2$ -values. In the region  $x < 0.1$  the ratios for  $F_2$  are larger than 0.98 for  $Q^2 > 50 \text{ GeV}^2$  and grow for larger values of  $x$ . Stronger deviations are observed for lower  $Q^2$  values. For  $F_L$  the corrections are larger. In the region  $x < 0.3$  and  $Q^2 > 100 \text{ GeV}^2$

the ratio is larger than 0.97, while for lower scales  $Q^2$  the deviations are larger. We limited the expansion to terms of  $\sim \mathcal{O}((m^2/Q^2)^2)$ , but higher order terms can be given straightforwardly. The expanded expressions do also allow direct Mellin transforms and provide a suitable analytic basis for Mellin-space programmes.<sup>3</sup>

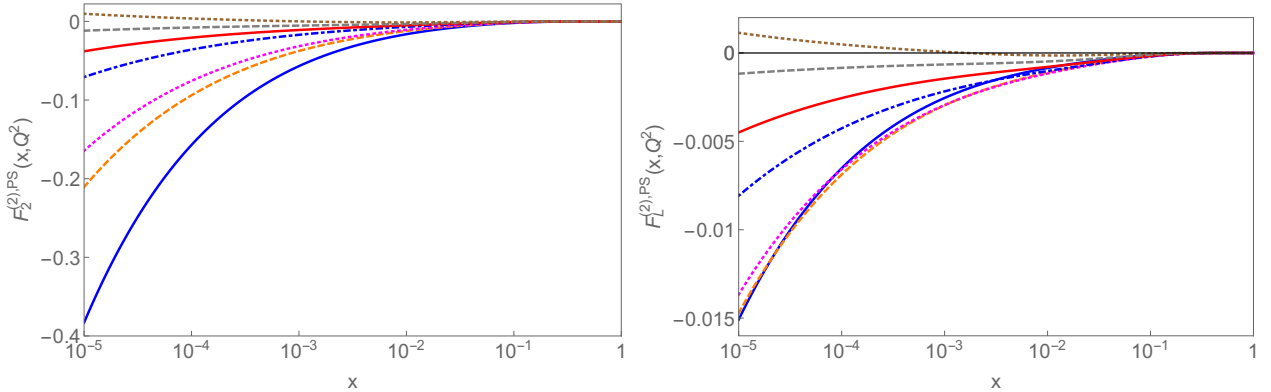


Figure 3.5.: The pure singlet contributions  $F_{2,q}^{(2),\text{PS}}$  (upper panel) and  $F_{L,q}^{(2),\text{PS}}$  (lower panel) for different values of  $Q^2$  and the scale choice  $\mu^2 = \mu_F^2 = Q^2$ . Full line (Blue):  $Q^2 = 10^4 \text{ GeV}^2$ ; dashed line (Orange):  $Q^2 = 10^3 \text{ GeV}^2$ ; dotted line (Magenta):  $Q^2 = 500 \text{ GeV}^2$ ; dash-dotted line (Blue):  $Q^2 = 100 \text{ GeV}^2$ ; full line (Red):  $Q^2 = 50 \text{ GeV}^2$ ; dashed line (Gray):  $Q^2 = 25 \text{ GeV}^2$ ; dotted line (Brown):  $Q^2 = 10 \text{ GeV}^2$ , using the parameterization of the parton distribution [207].

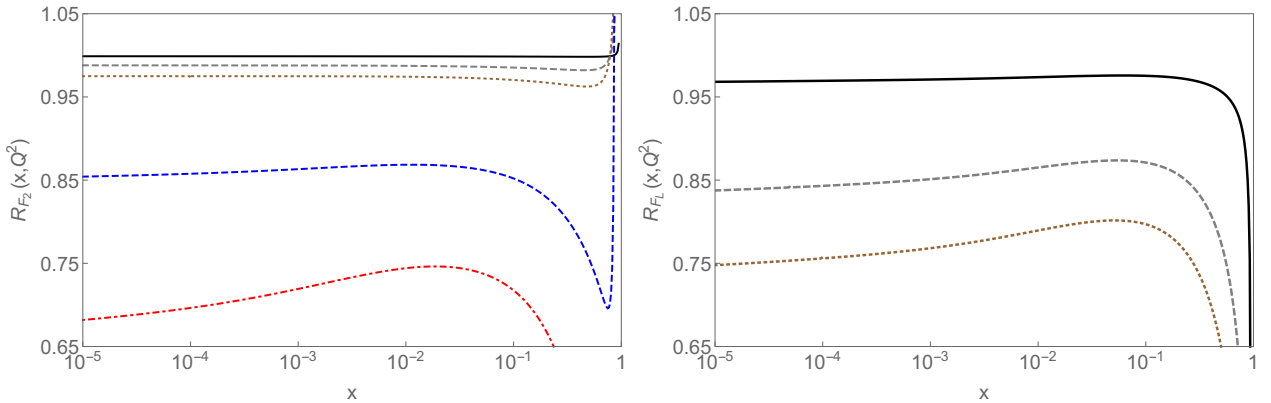


Figure 3.6.: The ratios of the structure functions  $F_{2,q}^{(2),\text{PS}}$  (left) and  $F_{L,q}^{(2),\text{PS}}$  (right) in the full calculation over the asymptotic approximation for different values of  $Q^2$  and the scale choice  $\mu^2 = \mu_F^2 = Q^2$ . Full line (Black):  $Q^2 = 10^4 \text{ GeV}^2$ ; dashed line (Gray):  $Q^2 = 10^3 \text{ GeV}^2$ ; dotted line (Brown):  $Q^2 = 500 \text{ GeV}^2$ ; lower dashed line (Blue):  $Q^2 = 100 \text{ GeV}^2$ ; dash-dotted line (Red):  $Q^2 = 50 \text{ GeV}^2$ , using the parameterization of the parton distribution [207]

In summary, we have calculated the massless and massive two-loop unpolarized pure singlet Wilson coefficients of deep-inelastic scattering for the structure functions  $F_2$  and  $F_L$ . In the massless case, we confirmed earlier analytic results in the literature, which can be expressed by harmonic polylogarithms. In the massive case, the Wilson coefficients are calculated analytically for the first

<sup>3</sup>In [299] precise numerical  $N$ -space implementations were given.

### 3. Unpolarized Pure-Singlet Wilson Coefficients at NLO

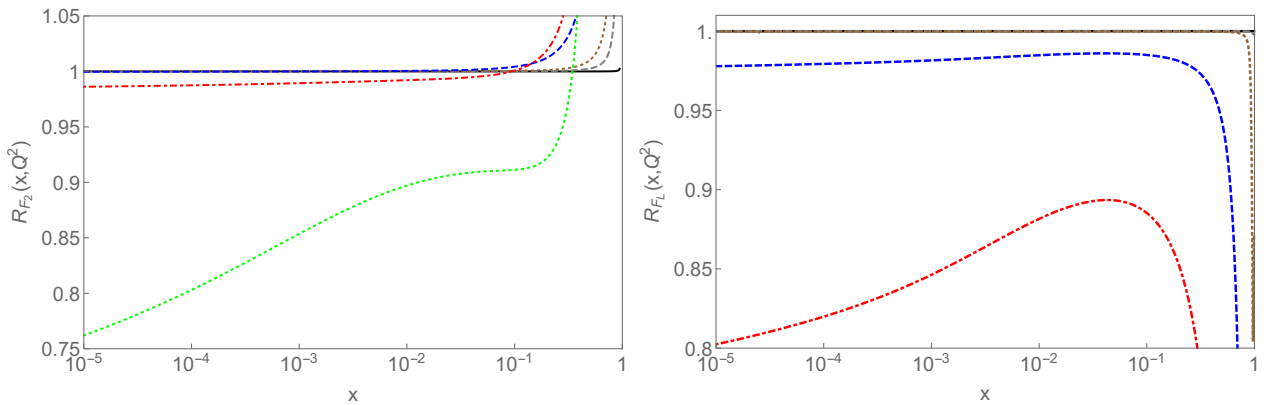


Figure 3.7.: The ratios of the structure functions  $F_{2,q}^{(2),\text{PS}}$  (left) and  $F_{L,q}^{(2),\text{PS}}$  (right) in the full calculation over the  $\mathcal{O}((m^2/Q^2)^2)$  improved approximation for different values of  $Q^2$  and the scale choice  $\mu^2 = \mu_F^2 = Q^2$ . Full lines (Black):  $Q^2 = 10^4 \text{ GeV}^2$ ; dashed lines (Gray):  $Q^2 = 10^3 \text{ GeV}^2$ ; dotted lines (Brown):  $Q^2 = 500 \text{ GeV}^2$ ; lower dashed lines (Blue):  $Q^2 = 100 \text{ GeV}^2$ ; dash-dotted lines (Red):  $Q^2 = 50 \text{ GeV}^2$ ; lower dotted lines (Green):  $Q^2 = 25 \text{ GeV}^2$ , using the parameterization of the parton distribution [207].

time. They are also given in terms of iterative integrals, including now, however, Kummer-elliptic integrals. The corresponding alphabets contain also elliptic letters. All integrals can be represented by classical (poly)logarithms with involved arguments with partly one more (elliptic) letter iterated upon. This representation is very well suited to obtain numerical results.

We have studied systematic expansions in the ratio  $m^2/Q^2$  in the asymptotic region and the velocity parameter  $\beta$  in the threshold region. In the former case the leading asymptotic result has been recovered, known from calculations based on massive OMEs and massless Wilson coefficients, proving asymptotic factorization in the present case. We have obtained a series of power corrections. Here the expansion coefficients are also spanned by harmonic polylogarithms. Retaining these terms extends the validity of the cross sections to lower scales of  $Q^2$ , which is relevant for experimental analyses. In particular, the predictions for the structure function  $F_L(x, Q^2)$  are significantly improved. In general, the Kummer-elliptic integrals, also obeying shuffling relations, span a wide class of iterative integrals which play a role as well in other multi-scale calculations.



## 4. Polarized Pure-Singlet Wilson Coefficients at NLO

Like in the previous section for the unpolarized case, the precise knowledge of the polarized structure functions is of importance to measure the polarized parton densities in high energy collisions and to determine, related to it, the strong coupling constant  $\alpha_s(M_Z)$  and the heavy quark masses, cf. [300]. The first two-loop QCD heavy flavor corrections to the polarized structure function  $g_1(x, Q^2)$  have been calculated in [173] in the asymptotic region  $Q^2 \gg m^2$ , where  $Q^2$  denotes the virtuality of the exchanged photon and  $m$  the mass of the heavy quark. The asymptotic two-loop QCD corrections have been recalculated in [175, 301, 302]. In [173] the region of low values of  $Q^2$  has been modeled by an ansatz. The leading threshold resummation for the gluonic contributions has been studied in [303]. The complete two-loop polarized heavy flavor Wilson coefficient in the non-singlet case has been calculated analytically in the tagged flavor case in [173] and for the complete contribution to the structure function  $g_1(x, Q^2)$  in [178], also completing former work on the polarized Bjorken sum rule in [304]. Numerical results for the polarized two-loop heavy flavor case have been given in [177] recently. Finally, in the non-singlet case the asymptotic contributions have been calculated to three-loop order analytically in [256, 305].

In this chapter we follow the previous one in the unpolarized case and calculate the polarized pure singlet two-loop heavy flavor corrections for the structure function  $g_1(x, Q^2)$  in the whole kinematic range analytically. We also compute the corresponding massless contributions, which have first been calculated in [306] and later in [307]. Since the calculations are carried out using dimensional regularization in  $d = 4 + \varepsilon$  dimensions one may work in the Larin scheme [209]<sup>1</sup> and perform, in the massless case, a finite renormalization to the  $M$ -scheme afterwards. The  $M$ -scheme is implicitly defined in Ref. [152] and restores the supersymmetric relation

$$\gamma_{qq}^{(n)} + \gamma_{gq}^{(n)} - \gamma_{qg}^{(n)} - \gamma_{gg}^{(n)} = 0 \quad (4.1)$$

between the anomalous dimensions up to 2-loop order. It is not known if this scheme is the same as the  $\overline{\text{MS}}$ -scheme. To proof this the Ward-identities of QCD have to be checked. We derive both the result in the asymptotic  $Q^2 \gg m^2$ , see also Refs. [173, 302], and in the threshold region. Numerical results are presented. Various technical aspects of the calculation can be found in the previous chapter and in Appendix D.

The chapter is organized as follows. In Section 4.1 we summarize basic relations for the polarized deep-inelastic scattering cross section. In Section 4.2 the result for the massless pure singlet Wilson coefficient  $C_{g_1}^{(2),\text{PS}}$  is presented. The recalculation of the massless Wilson coefficient is necessary, since in Ref. [306] different schemes have been used in part. The corresponding massive Wilson coefficient is calculated in Section 4.3. The corresponding results for the twist-2 contributions to the structure function  $g_2(x, Q^2)$  can be obtained by using the Wandzura-Wilczek relation [162], as has been shown for the massless quarkonic [233, 277–279] and gluonic [174] cases, for diffractive scattering [308], non-forward scattering [309], and the target mass corrections [228, 229]. Limiting cases are studied in Section 4.4 and numerical results are presented in Section 4.5. Some Mellin convolutions appearing due to renormalization are listed in Appendix D.4.

<sup>1</sup>For other  $\gamma_5$  schemes see Refs. [56, 210–212, 245–248].

### 4.1. The Deep-inelastic Scattering Cross Section in the Polarized Case

The scattering cross sections for deep-inelastic charged lepton scattering of polarized nucleons are obtained polarizing the incoming lepton longitudinally and the target nucleon either longitudinally or transversally, resulting into the spin 4-vectors  $S_L$  and  $S_T$ ,

$$S_L = (0, 0, 0; M) \quad (4.2)$$

$$S_T = M(0, \cos(\beta), \sin(\beta); 0) \quad (4.3)$$

in the nucleon rest frame. One has  $S_L \cdot p = S_T \cdot p = 0$ , with  $p$  the nucleon 4-momentum. The scattering cross sections are given by, cf. e.g. [228, 310],

$$\frac{d^2\sigma(\lambda, \pm S_L)}{dxdy} = \pm 2\pi S \left[ -2\lambda y \left( 2 - y - \frac{2xyM^2}{S} \right) xg_1(x, Q^2) + 8\lambda \frac{yxM^2}{S} xg_2(x, Q^2) \right] \quad (4.4)$$

$$\begin{aligned} \frac{d^3\sigma(\lambda, \pm S_T)}{dxdyd\phi} &= \pm S \frac{\alpha^2}{Q^4} 2\sqrt{\frac{M^2}{S}} \sqrt{xy \left[ 1 - y - \frac{xyM^2}{S} \right]} \cos(\beta - \phi) \\ &\times [-2\lambda y x g_1(x, Q^2) - 4\lambda x g_2(x, Q^2)] \end{aligned} \quad (4.5)$$

for pure virtual photon exchange. Here  $S$  denotes the energy of the process in the centre-of-mass system,  $M$  is the nucleon mass,  $\lambda$  the degree of lepton polarization,  $\alpha = e^2/(4\pi)$  is the fine structure constant,  $Q^2 = -q^2$  denotes the photon virtuality and  $x = Q^2/(Sy)$ ,  $y = l \cdot q / p \cdot q$  are the Bjorken variables with  $l$  the incoming charged lepton and proton momenta,  $S = (p+l)^2$  and  $\phi$  is the azimuthal angle of the final state lepton, which can be integrated over in the case of longitudinal polarization as introduced in Chapter 2.

In the following we will present a series of relations in Mellin- $N$  space for convenience. The respective quantities in momentum-fraction  $z$ -space are related to those in Mellin-space by the Mellin transformation, cf. Eq. (2.45). The structure function  $g_1(N, Q^2)$  is given in the twist-2 approximation using the factorization theorems [311–319] by

$$\begin{aligned} g_1(N, Q^2) &= \frac{1}{2} \left[ \frac{1}{N_F} \sum_{k=0}^{N_F} e_k^2 \left\{ \Sigma(N, \mu_F^2) C_q^{\text{PS}} \left( N, \frac{Q^2}{\mu_F^2} \right) + G(N, \mu_F^2) C_g^{\text{S}} \left( N, \frac{Q^2}{\mu_F^2} \right) \right\} \right. \\ &\quad \left. + \Delta(N, \mu_F^2) C_q^{\text{NS}} \left( N, \frac{Q^2}{\mu_F^2} \right) \right]. \end{aligned} \quad (4.6)$$

Here

$$\Sigma(N) = \sum_{k=1}^{N_F} [\Delta q(N) + \Delta \bar{q}(N)] \quad (4.7)$$

denotes the polarized singlet distribution,  $G(N)$  the polarized gluon distribution,  $\Delta(N)$  the polarized flavor non-singlet distribution

$$\Delta(N) = \sum_{i=1}^{N_F} \left[ e_i^2 - \frac{1}{N_F} \sum_{k=1}^{N_F} e_k^2 \right] [\Delta q_i(N) + \Delta \bar{q}_i(N)]. \quad (4.8)$$

$e_k$  labels the electric charge of the  $k$ th light quark and  $\Delta q_i$  ( $\Delta \bar{q}_i$ ) are the polarized parton distributions of the  $i$ th light quark (anti-quark).

At twist-2 the Mellin transform of the structure function  $g_2$  is related to that of  $g_1$  by

$$g_2(N, Q^2) = -\frac{N-1}{N} g_1(N, Q^2) \quad (4.9)$$

or

$$g_2(x, Q^2) = -g_1(x, Q^2) + \int_0^1 \frac{dy}{y} g_1(y, Q^2). \quad (4.10)$$

Note that in the massive pure-singlet case the support of both structure functions is limited by  $0 < x < 1/(1 + 4m^2/Q^2)$  due to the production of two heavy quarks.

The different steps in the renormalization and factorization of the polarized massless Wilson coefficients have been described in [131, 306] and for the massive Wilson coefficients in [302] using the Larin scheme. The calculation of the Wilson coefficient will also be performed in the Larin scheme, i.e. identifying

$$\gamma_5 = \frac{i}{24} \gamma_\mu \gamma_\nu \gamma_\rho \gamma_\delta \epsilon^{\mu\nu\rho\delta} \quad (4.11)$$

and performing the result contraction of two Levi-Civita tensors in  $d$  dimensions (2.87). In the present case the finite renormalization moving to the  $M$ -scheme only affects the massless Wilson coefficient by adding the term  $-z_{\text{PS}}^{(2)}$ , Eq. (4.34). More details regarding the finite renormalization will be given in the next section.

## 4.2. The Massless Wilson Coefficient

The Feynman diagrams contributing to the polarized massless two-loop Wilson coefficient are shown in Fig. D.1. Here all quark lines are massless. The massless resp. massive Wilson coefficients are obtained following Ref. [306], Eqs. (3.7–3.18). The corresponding phase space parametrization can be found in Appendix D. We apply the Larin scheme [209] in which the contraction of the free indices of the two appearing Levi-Civita tensors have to be performed in  $d$  dimensions.

The unrenormalized two-loop massless pure singlet Wilson coefficient reads in Mellin- $N$  space

$$\hat{C}_{g_1}^{(2),\text{PS}} = \hat{a}_s^2 S_\varepsilon^2 \left( \frac{Q^2}{\mu^2} \right)^\varepsilon \left\{ \frac{1}{\varepsilon^2} \frac{1}{2} P_{qg}^{(0)} P_{gq}^{(0)} + \frac{1}{\varepsilon} \left[ \frac{1}{2} P_{qq}^{(1),\text{PS}} + P_{gq}^{(0)} \bar{c}_{g_1,g}^{(1)} \right] + \bar{c}_{g_1,q}^{(2),\text{PS}} + P_{qg}^{(0)} a_{g_1,g}^{(1)} \right\}, \quad (4.12)$$

where  $\hat{a}_s = \hat{g}_s^2/(4\pi)^2$  denotes the unrenormalized strong coupling constant and  $S_\varepsilon$  the spherical factor, cf. Eq. (G.17).  $\bar{c}_i^{(k)}$  and  $a_{g_1,g}^{(1)}$  are the expansion coefficients of the one-loop Wilson coefficient with

$$\hat{C}_{g_1,g}^{(1)} = \hat{a}_s S_\varepsilon \left( \frac{Q^2}{\mu^2} \right)^{\varepsilon/2} \left[ \frac{1}{\varepsilon} P_{qg} + \bar{c}_{g_1,g}^{(1)} + \varepsilon a_{g_1,g}^{(1)} \right], \quad (4.13)$$

given by the Feynman diagrams in Fig. 3.1, where all quark lines are massless. One obtains

$$\bar{c}_{g_1,g}^{(1)} = 4T_F N_F \left[ -(2z-1)[H_1 + H_0] + 3 - 4z \right], \quad (4.14)$$

$$a_{g_1,g}^{(1)} = T_F N_F \left[ -12 + 16z + 3(1-2z)\zeta_2 - (6-8z)(H_0 + H_1) - (1-2z)(H_0 + H_1)^2 \right]. \quad (4.15)$$

The contributing splitting functions [96, 153–157] are

$$P_{qg}(z) = 8T_F N_F \left[ z^2 - (1-z)^2 \right], \quad (4.16)$$

$$P_{gq}(z) = 4C_F \frac{1 - (1-z)^2}{z}, \quad (4.17)$$

$$P_{qq}^{(1),\text{PS}}(z) = 16C_F T_F N_F \left[ 1 - z - (1-3z)H_0 - (1+z)H_0^2 \right], \quad (4.18)$$

#### 4. Polarized Pure-Singlet Wilson Coefficients at NLO

see Appendix A for the definition of the color factors. Also in this chapter we will use the conventions introduced in Eq. (3.12). The harmonic polylogarithms we will use in the following are introduced in Appendix C.4. Again, we use the shorthand notation  $H_{\bar{a}}(z) \equiv H_{\bar{a}}$  in case of the argument  $z$  if not stated otherwise. The harmonic polylogarithms are dual to the harmonic sums [149, 150] by the Mellin transformation, cf. Eq. (2.45).

In the Larin scheme we obtain

$$\begin{aligned}
\hat{C}_{g_1}^{(2),\text{PS},L} &= -C_F T_F N_F \left\{ -\frac{1}{\varepsilon^2} [80(1-z) + 32(1+z)H_0] + \frac{1}{\varepsilon} [184(1-z) - 32(1+z)\zeta_2 \right. \\
&\quad + 40(3-z)H_0 + 24(1+z)H_0^2 + 80(1-z)H_1 + 32(1+z)H_{0,1}] - \frac{1432}{3}(1-z) \\
&\quad - \frac{4}{3}(233 - 43z)H_0 + \frac{32(1+z)^3}{3z}H_{-1}H_0 - \frac{2}{3}(129 - 15z + 8z^2)H_0^2 \\
&\quad - \frac{28}{3}(1+z)H_0^3 - (1-z)[184 + 80H_0]H_1 - 40(1-z)H_1^2 - (1+z)[40 + 32H_0]H_{0,1} \\
&\quad - \frac{32(1+z)^3}{3z}H_{0,-1} + 16(1+z)[H_{0,0,1} - 2H_{0,1,1}] \\
&\quad \left. + \left[ \frac{4}{3}(129 - 45z + 8z^2) + 56(1+z)H_0 \right] \zeta_2 + 16(1+z)\zeta_3, \right. \tag{4.19}
\end{aligned}$$

performing the phase space integrations as has been outlined in [5, 131], cf. Appendix D. We agree with the result obtained in the original Ref. [306], where the result has been obtained in the Larin scheme. The Erratum to Ref. [306] introduces the finite renormalization to the  $M$ -scheme.

At  $\mathcal{O}(a_s^2)$  the renormalization of the coupling constant does not contribute. The poles in  $\varepsilon$  in Eq. (4.19) are due to collinear singularities only, which have to be factorized. One may proceed as follows. The unfactorized quarkonic Wilson coefficients for the structure function  $g_1$ ,  $\hat{C}_{1,q}^{\text{NS,S}}$  in Mellin-space are

$$\hat{C}_{1,q}^{\text{NS}} = \Gamma_{qq}^{\text{NS}} C_q^{\text{NS}} \tag{4.20}$$

$$\hat{C}_{1,q}^{\text{S}} = \Gamma_{qq}^{\text{S}} C_q^{\text{S}} + \Gamma_{gq}^{\text{S}} C_g^{\text{S}}. \tag{4.21}$$

The pure singlet contribution is obtained by

$$\begin{aligned}
\hat{C}_{1,q}^{\text{PS}} &= \hat{C}_{1,q}^{\text{S}} - \hat{C}_{1,q}^{\text{NS}} \\
&= \Gamma_{qq}^{\text{S}} C_q^{\text{S}} - \Gamma_{qq}^{\text{NS}} C_q^{\text{NS}} + \Gamma_{gq}^{\text{S}} C_g^{\text{S}} \tag{4.22}
\end{aligned}$$

$$= \left[ \Gamma_{qq}^{\text{NS}} + \Gamma_{qq}^{\text{S}} \right] \left[ C_q^{\text{NS}} + C_q^{\text{PS}} \right] - \Gamma_{qq}^{\text{NS}} C_q^{\text{NS}} + \Gamma_{gq}^{\text{S}} C_g^{\text{S}} \tag{4.23}$$

with

$$\Gamma_{gq}^{(0)} = \hat{a}_s S_\varepsilon \left( \frac{\mu_F^2}{\mu^2} \right)^{\varepsilon/2} \frac{1}{\varepsilon} P_{gq}^{(0)}, \tag{4.24}$$

$$\Gamma_{qq}^{(1),\text{PS}} = \hat{a}_s^2 S_\varepsilon^2 \left( \frac{\mu_F^2}{\mu^2} \right)^\varepsilon \left[ \frac{1}{\varepsilon^2} P_{qg}^{(0)} P_{gq}^{(0)} + \frac{1}{\varepsilon} P_{qq}^{(1),\text{PS}} \right]. \tag{4.25}$$

and

$$\hat{C}_{1,q}^{\text{PS}} = a_s^2 \left\{ \frac{1}{\varepsilon^2} \frac{1}{2} P_{qg}^{(0)} P_{gq}^{(0)} + \frac{1}{\varepsilon} \left[ \frac{1}{2} P_{qq}^{(1),\text{PS}} + P_{gq}^{(0)} C_g^{(1)} \right] + C_q^{(2),\text{PS}} \right\}. \tag{4.26}$$

The factorized massless pure singlet two-loop Wilson coefficient  $C_{g_1}^{(2),\text{PS},L}$  is given by

$$C_{g_1}^{(2),\text{PS},L} \left( z, \frac{Q^2}{\mu^2} \right) = a_s^2 \left\{ \frac{1}{8} P_{qq}^{(0)} P_{gq}^{(0)} L_M^2 + \frac{1}{2} \left[ P_{qq}^{(1),\text{PS}} + P_{gq}^{(0)} \bar{c}_g^{(1)} \right] L_M + \bar{c}_q^{(2),\text{PS}} \right\}, \quad (4.27)$$

where

$$L_M = \ln \left( \frac{Q^2}{\mu} \right). \quad (4.28)$$

Here we set  $\mu_F = \mu$ , and work with a single scale for factorization and renormalization. Note that the splitting function  $P_{qq}^{(1),\text{PS}}$  is correctly obtained, cf. Refs. [155–157], despite working in the Larin scheme, cf. also Ref. [158].

The massless Wilson coefficient in the  $M$ -scheme is obtained by a factorization scheme transformation, cf. Ref. [158]. Since the structure function is given by the convolution of the Wilson coefficients with the PDFs, we can introduce a finite rotation between them. The explicit relations read

$$\begin{aligned} g_1^{\text{NS}} &= C_{g_1}^{\text{NS},L} \Delta_L = \left[ C_{g_1}^{\text{NS},L} (Z^{\text{NS}})^{-1} \right] \left[ Z^{\text{NS}} \Delta_L \right] \\ &\equiv C_{g_1}^{\text{NS},M} \Delta_M, \end{aligned} \quad (4.29)$$

$$\begin{aligned} \begin{pmatrix} g_1^{\text{S}} \\ g_{1,g} \end{pmatrix} &= \begin{pmatrix} C_{g_1}^{\text{S},L} \\ C_{g_{1,g}}^{\text{L}} \end{pmatrix} \cdot \begin{pmatrix} \Sigma_L \\ G_L \end{pmatrix} = \left[ \begin{pmatrix} C_{g_1}^{\text{S},L} \\ C_{g_{1,g}}^{\text{L}} \end{pmatrix} \cdot (Z^{\text{S}})^{-1} \right] \cdot \left[ Z^{\text{S}} \cdot \begin{pmatrix} \Sigma_L \\ G_L \end{pmatrix} \right] \\ &\equiv \begin{pmatrix} C_{g_1}^{\text{S},M} \\ C_{g_{1,g}}^{\text{M}} \end{pmatrix} \cdot \begin{pmatrix} \Sigma_M \\ G_M \end{pmatrix}. \end{aligned} \quad (4.30)$$

The perturbative expansion of the transformations, which transform from the Larin into the  $M$ -scheme, are given by [152]

$$Z^{\text{NS}} = 1 + a_s z_{qq}^{(1)} + a_s^2 z_{qq}^{(2),\text{NS}} + \mathcal{O}(a_s^3), \quad (4.31)$$

$$Z^{\text{S}} = 1 + a_s \begin{pmatrix} z_{qq}^{(1)} & 0 \\ 0 & 0 \end{pmatrix} + a_s^2 \begin{pmatrix} z_{qq}^{(2),\text{NS}} + z_{qq}^{(2),\text{PS}} & 0 \\ 0 & 0 \end{pmatrix} + \mathcal{O}(a_s^3). \quad (4.32)$$

Using this prescription we arrive at the following finite renormalization for the pure singlet Wilson coefficient

$$C_{g_1}^{(2),\text{PS},M} = C_{g_1}^{(2),\text{S},M} - C_{g_1}^{(2),\text{NS},M} = C_{g_1}^{(2),\text{PS},L} - z_{\text{PS}}^{(2)}, \quad (4.33)$$

with [152]

$$z_{\text{PS}}^{(2)} = C_F T_F N_F \left[ 16(1-z) + 8(3-z)H_0 + 4(2+z)H_0^2 \right], \quad (4.34)$$

cf. [158, 302].  $C_{g_1}^{(2),\text{PS},M}$  in  $z$ -space is given by

$$\begin{aligned} C_{g_1}^{(2),\text{PS},M} \left( z, \frac{Q^2}{\mu^2} \right) &= a_s^2 C_F T_F N_F \left\{ [20(1-z) + 8(1+z)H_0] L_M^2 - [(1-z)(88 + 40H_1) \right. \\ &\quad \left. + 16(1+z)(H_0^2 + H_{0,1} - \zeta_2) + 32(2-z)H_0] L_M + \frac{760}{3}(1-z) \right. \\ &\quad \left. + \frac{4}{3}(119 - 13z)H_0 - \frac{32(1+z)^3}{3z} H_{-1} H_0 + \frac{2}{3}[75 - 15z + 8z^2] H_0^2 \right\} \end{aligned}$$

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$$\begin{aligned}
& + \frac{20}{3}(1+z)\mathbf{H}_0^3 + (1-z)(88+40\mathbf{H}_0)\mathbf{H}_1 + 20(1-z)\mathbf{H}_1^2 + [8(3+z) \\
& + 16(1+z)\mathbf{H}_0]\mathbf{H}_{0,1} + \frac{32(1+z)^3}{3z}\mathbf{H}_{0,-1} + 16(1+z)\mathbf{H}_{0,1,1} \\
& - 32 \left[ \frac{1}{3}(9-3z+z^2) + (1+z)\mathbf{H}_0 \right] \zeta_2 - 16(1+z)\zeta_3 \Big\}. \tag{4.35}
\end{aligned}$$

We agree with the result given in the last Erratum to Ref. [306] where the additional scheme transformation to the  $M$ -scheme has been applied.

### 4.3. The Massive Wilson Coefficient

The kinematic domain for the massive Wilson coefficient is given by

$$0 < z < \frac{Q^2}{4m^2 + Q^2}. \tag{4.36}$$

The unrenormalized two-loop massive pure singlet Wilson coefficient reads in Mellin- $N$  space

$$\hat{H}_{g_1}^{(2),\text{PS},L} = \hat{a}_s^2 S_\varepsilon^2 \left( \frac{Q^2}{\mu^2} \right)^\varepsilon \left\{ \frac{1}{\varepsilon} P_{gq}^{(0)} h_{g_1,g}^{(1)} + h_{g_1,q}^{(2),\text{PS},L} + P_{qg}^{(0)} \bar{b}_{g_1,g}^{(1)} \right\}. \tag{4.37}$$

The contributing Feynman diagrams are shown in Fig. D.1, where now the outgoing quark lines with momenta  $k_1$  and  $k_2$  are taken massive. Here  $h_{g_1,g}^{(1)}$  [161, 171, 172] and  $\bar{b}_{g_1,g}^{(1)}$  are the expansion coefficients of the one-loop Wilson coefficient

$$\hat{H}_{g_1,g}^{(1)} = \hat{a}_s S_\varepsilon \left( \frac{Q^2}{\mu^2} \right)^{\varepsilon/2} \left[ h_{g_1,g}^{(1)} + \varepsilon \bar{b}_{g_1,g}^{(1)} \right] \tag{4.38}$$

given by the diagrams in Fig. 3.1 now with massive quark lines. The expansion coefficients are given in  $z$ -space by

$$h_{g_1,g}^{(1)} = 4T_F \left[ (3-4z)\beta - (1-2z)\mathbf{H}_0 \left( \frac{1+\beta}{1-\beta} \right) \right] \tag{4.39}$$

$$\begin{aligned}
\bar{b}_{g_1,g}^{(1)} &= T_F \left\{ -4(3-4z)\beta + (1-2z)\mathbf{H}_0^2 \left( \frac{1-\beta}{1+\beta} \right) - 2 \left[ (3-4z)\beta + (1-2z)\mathbf{H}_0 \left( \frac{1-\beta}{1+\beta} \right) \right] \right. \\
&\quad \left. \times [\mathbf{H}_0 + \mathbf{H}_1 - 2\ln(\beta)] + 4(1-2z)\mathbf{H}_{0,1} \left( \frac{2\beta}{1+\beta} \right) \right\}. \tag{4.40}
\end{aligned}$$

Here  $\beta$  denotes the velocity of the produced heavy quarks,

$$\beta = \sqrt{1 - \frac{4m^2}{Q^2} \frac{z}{1-z}}. \tag{4.41}$$

Since the two heavy quarks do not induce collinear divergences the mass factorization in the massive case reads

$$\hat{H}_{g_1}^{(2),\text{PS},L} = H_{g_1}^{(2),\text{PS}} + \Gamma_{gq} \otimes H_{g_1,g}^{(1),\text{PS}}. \tag{4.42}$$

We find

$$H_{g_1}^{(2),\text{PS},L} = \hat{a}_s^2 S_\varepsilon^2 \left\{ \left( \frac{Q^2}{\mu^2} \right)^\varepsilon \left[ \frac{1}{\varepsilon} P_{gq}^{(0)} \otimes h_{g_1}^{(1)} + h_{g_1}^{(2),\text{PS}} + P_{gq}^{(0)} \otimes \bar{b}_{g_1}^{(1)} \right] \right\}$$

$$- \left( \frac{\mu_F^2}{\mu^2} \right)^{\varepsilon/2} \left( \frac{Q^2}{\mu^2} \right)^{\varepsilon/2} \left[ \frac{1}{\varepsilon} P_{gq}^{(0)} \otimes h_{g_1}^{(1)} + P_{gq}^{(0)} \otimes \bar{b}_{g_1}^{(1)} \right]. \quad (4.43)$$

Identifying the renormalization and factorization scale,  $\mu = \mu_F$ , we finally obtain

$$H_{g_1}^{(2),\text{PS}} = a_s^2 \left[ \frac{1}{2} P_{gq}^{(0)} \otimes h_{g_1}^{(1)} L_M + h_{g_1}^{(2),\text{PS}} \right] + \mathcal{O}(\varepsilon). \quad (4.44)$$

Note that in the pure singlet case neither the heavy quark mass nor the coupling constant is renormalized at two-loop order.

The massive pure singlet Wilson coefficient is obtained as a four-fold integral over two angular and two energy variables, cf. Chapter 3 and Appendix D for details of the calculation. These integrals are systematically turned into iterative integrals. This process leads to a set of letters, through which these integrals are defined, see also [241]. It turns out that the polarized structure functions can be expressed with the same alphabet as the unpolarized ones, cf. Eqs. (3.40-3.51). These iterative integrals have maximally weight  $w = 3$  and belong to the Kummer-elliptic integrals, cf. Eq. (3.58), in general. The variable  $k$  is defined by

$$k = \frac{\sqrt{z}}{\sqrt{1 - (1 - z)\beta^2}}. \quad (4.45)$$

One obtains for the following analytic result of the massive polarized two-loop Wilson coefficient

$$\begin{aligned} H_{g_1}^{(2),\text{PS},L} = & C_F T_F \left\{ -\frac{16(1-z)P_{67}}{3k^2} \left\{ \mathbf{H}_{w_5,0} - \mathbf{H}_{w_6,0} + \mathbf{H}_{w_7,0} - \mathbf{H}_{w_8,0} - [\mathbf{H}_{w_5} - \mathbf{H}_{w_6} + \mathbf{H}_{w_7} - \mathbf{H}_{w_8}] \right. \right. \\ & \times \mathbf{H}_0 \left. \right\} - \frac{8P_{68}}{3k^2} \mathbf{H}_{w_2,-1} - \frac{8P_{69}}{3k^2} \mathbf{H}_1 \mathbf{H}_{w_1} + \frac{4(1-z)P_{70}}{3k^2 z} \left\{ \mathbf{H}_{w_6,1} - \mathbf{H}_{w_8,-1} - \mathbf{H}_{w_6} \mathbf{H}_1 \right. \\ & \left. + \mathbf{H}_{w_8} \mathbf{H}_{-1} \right\} - \frac{4(1-z)P_{71}}{3k^2 z} \left\{ \mathbf{H}_{w_6,-1} - \mathbf{H}_{w_8,1} + \mathbf{H}_{w_8} \mathbf{H}_1 - \mathbf{H}_{w_6} \mathbf{H}_{-1} \right\} \\ & + \frac{4(1-z)P_{72}}{3k^2 z} \left\{ \mathbf{H}_{w_5,-1} - \mathbf{H}_{w_7,1} + \mathbf{H}_{w_7} \mathbf{H}_1 - \mathbf{H}_{w_5} \mathbf{H}_{-1} \right\} - \frac{4(1-z)P_{73}}{3k^2 z} \left\{ \mathbf{H}_{w_5,1} \right. \\ & \left. - \mathbf{H}_{w_7,-1} - \mathbf{H}_{w_5} \mathbf{H}_1 + \mathbf{H}_{w_7} \mathbf{H}_{-1} \right\} + \frac{16P_{74}}{3(1-k\beta)} \mathbf{H}_{w_1} - \frac{16P_{75}}{3(1+k\beta)} \mathbf{H}_{w_2} \\ & + \frac{8(1-z)P_{76}}{3(k(2-z)-z)(1-k\beta)} \mathbf{H}_{w_5} + \frac{8(1-z)P_{77}}{3(k(2-z)+z)(1+k\beta)} \mathbf{H}_{w_6} \\ & - \frac{8(1-z)P_{78}}{3(k(2-z)-z)(1+k\beta)} \mathbf{H}_{w_7} - \frac{8(1-z)P_{79}}{3(k(2-z)+z)(1-k\beta)} \mathbf{H}_{w_8} \\ & + \frac{32P_{80}}{3k^2(k^2(2-z)^2-z^2)} \mathbf{H}_1 - \frac{32P_{81}}{3k^2(k^2(2-z)^2-z^2)} \mathbf{H}_{-1} \\ & + \frac{1216}{3} (1-z)\beta + 8(1-z)(1-2z) [\mathbf{H}_1 + \mathbf{H}_{-1} - 2\beta] (\ln(z) + \ln(1-z)) \\ & + 16(1+2z) \left\{ 2(\mathbf{H}_{w_1,w_4} + \mathbf{H}_{w_2,w_4} + \mathbf{H}_{w_3,w_1} + \mathbf{H}_{w_3,w_2}) \right. \\ & + k(\mathbf{H}_{w_1}^2 - \mathbf{H}_{w_2}^2) + [-2\ln(k^2-z) + 6\ln(k) - \ln(1-k^2) + \ln(k^2-z^2) - 2\mathbf{H}_{w_3}] \\ & \times (\mathbf{H}_{w_1} + \mathbf{H}_{w_2}) + k(1-z) [\mathbf{H}_{w_5,w_1} + \mathbf{H}_{w_6,w_2} - \mathbf{H}_{w_7,w_2} - \mathbf{H}_{w_8,w_1}] \\ & \left. - k(1-z) [\mathbf{H}_{w_5} - \mathbf{H}_{w_8}] \mathbf{H}_{w_1} - k(1-z) [\mathbf{H}_{w_6} - \mathbf{H}_{w_7}] \mathbf{H}_{w_2} \right\} \\ & + 16(1-z)(7-2z)\beta \ln(k^2-z^2) + 8 \left( 7 - \left( 2 - \frac{1}{k^2} \right) z \right) \left\{ 2\mathbf{H}_1 \mathbf{H}_0 - 6\ln(k) \mathbf{H}_1 \right. \end{aligned}$$

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$$\begin{aligned}
& + \ln(1 - k^2)H_1 + 2 \ln(k^2 - z)H_1 + 2H_{w_3}H_1 - 6 \ln(k)H_{-1} + \ln(1 - k^2)H_{-1} \\
& + 2 \ln(k^2 - z)H_{-1} + 2H_{-1}H_{w_3} - 2H_{0,1} - 2H_{1,w_4} - 2H_{w_3,1} - 2H_{w_3,-1} + 2H_{-1,0} \\
& - 2H_{-1,w_4} \left. \right\} + \frac{32}{3} \left( -3k^2 + \frac{z^2}{k^2} - 3(1 + z^2) \right) [H_{w_1} + H_{w_2}]H_0 + 8 \ln(k^2 - z^2) \\
& \times \left( -8 + \frac{(-1 + 5k^2)z}{k^2} - 2z^2 \right) [H_1 + H_{-1}] + \frac{8}{3} \left( 6k^2 - \frac{3z}{k} - \frac{2z^2}{k^2} + 6(2 + 2z \right. \\
& \left. + z^2) - 3k(8 - 5z + 2z^2) \right) [H_{w_1}H_{-1} - H_{w_2}H_1] + \frac{8}{3} \left( 6k^2 + \frac{3z}{k} - \frac{2z^2}{k^2} + 6(2 + 2z \right. \\
& \left. + z^2) + 3k(8 - 5z + 2z^2) \right) H_{w_2}H_{-1} + \frac{4}{3} \left( 87 + \frac{4}{z} - \frac{9(-1 + 2k^2)z}{k^2} \right) [H_1^2 - H_{-1}^2] \\
& - \frac{16}{3} k(1 - z)(3 + 2z + 3z^2) \left\{ \frac{1}{\sqrt{z}} [H_{w_{10},w_5} - H_{w_{10},w_6} + H_{w_{10},w_7} - H_{w_{10},w_8}] \right. \\
& \left. - \frac{k}{\sqrt{z}} \left( H_{w_5,w_{11}} + H_{w_6,w_{11}} + H_{w_7,w_{11}} + H_{w_8,w_{11}} - [H_{w_5} + H_{w_6} + H_{w_7} + H_{w_8}]H_{w_{11}} \right) \right. \\
& \left. - 2k(1 - k^2)\sqrt{z} \left( H_{w_5,w_{12}} + H_{w_6,w_{12}} + H_{w_7,w_{12}} + H_{w_8,w_{12}} - [H_{w_5} + H_{w_6} + H_{w_7} \right. \right. \\
& \left. \left. + H_{w_8}]H_{w_{12}} \right) - \frac{2}{\sqrt{z}(1 - z)} [H_{w_{10},w_1} + H_{w_{10},w_2}] - \frac{2(1 - k^2)\sqrt{z}}{1 - z} [H_{w_{12},1} \right. \\
& \left. + H_{w_{12},-1}] \right\} - \frac{384(k^2 - z)}{k^2\beta} H_{w_3} - \frac{8}{3} \left( 39 - \frac{4}{z} + \frac{9(1 - 2k^2)z}{k^2} \right) H_{-1}H_1 \\
& + 32 \left( k^2 - (2 - z)z - \frac{z^2}{3k^2} \right) H_{w_{1,0}} + \frac{8}{3} \left( 6k^2 + \frac{3z}{k} - \frac{2z^2}{k^2} - 3kz(1 - 2z) \right. \\
& \left. - 6(1 + 4z - z^2) \right) H_{w_{1,1}} + \frac{8}{3} \left( 6 - 6k^2 + 24z + \frac{3z}{k} - 6z^2 + \frac{2z^2}{k^2} \right. \\
& \left. - 3kz(1 - 2z) \right) H_{w_{1,-1}} + 32 \left( k^2 - (2 - z)z - \frac{z^2}{3k^2} \right) H_{w_{2,0}} + \frac{8}{3} \left( 6k^2 - \frac{3z}{k} \right. \\
& \left. + 3k(1 - 2z)z - \frac{2z^2}{k^2} - 6(1 + 4z - z^2) \right) H_{w_{2,1}} + \left( 208 - \frac{64}{3z} + \frac{48(1 - 2k^2)z}{k^2} \right) \\
& \times H_{-1,1} - \frac{64k^2(1 - z^2)(1 + 3z^2)}{3z} \left\{ H_{w_9,1} + H_{w_9,-1} - k(1 - z) [H_{w_9,w_5} + H_{w_9,w_6} \right. \\
& \left. + H_{w_9,w_7} + H_{w_9,w_8}] \right\} + 8(1 + z) \left\{ -4H_{0,1,1} - 4H_{0,-1,1} + 20H_{1,1,1} + 4H_{1,1,w_4} \right. \\
& + 4H_{1,-1,w_4} - 4H_{w_3,1,1} + 4H_{w_3,1,-1} - 4H_{w_3,-1,1} + 4H_{w_3,-1,-1} + 4H_{-1,1,0} \\
& + 16H_{-1,1,1} - 4H_{-1,1,w_4} + 4H_{-1,-1,0} + 16H_{-1,-1,1} - 4H_{-1,-1,w_4} + 20H_{-1,-1,-1} \\
& + \left( \ln(1 - k^2) - \ln(k^2 - z^2) + 2 \ln(k^2 - z) - 6 \ln(k) \right) [H_{-1}^2 - H_1^2 - 2H_1H_{-1} \\
& + 4H_{-1,1}] + [(10H_{-1} - 4H_{w_3})H_1 - 4H_0H_1 + 2H_1^2 - 2H_{1,1} - 4H_{w_3,1} - 4H_{w_3,-1} \\
& - 12H_{-1,1} - 10H_{-1,-1}]H_{-1} + [4H_{1,1} + 8H_{-1,1} + 4H_{-1,-1} - 4H_1^2]H_{w_3} + [4H_{0,1} \\
& + 4H_{0,-1} - 10H_{1,1} + 4H_{w_3,1} + 4H_{w_3,-1} - 4H_{-1,1} - 10H_{-1,-1}]H_1 \\
& + [-4H_1^2 + 4H_{1,1} + 4H_{-1,1}]H_0 \left. \right\} + 32k(1 + z) \left\{ H_{w_1,1,0} + H_{w_1,1,1} - H_{w_1,1,w_4} \right. \\
& - H_{w_1,1,-1} + H_{w_1,-1,0} + H_{w_1,-1,1} - H_{w_1,-1,w_4} - H_{w_1,-1,-1} - H_{w_2,1,0} - H_{w_2,1,1} \\
& \left. + H_{w_2,1,w_4} + H_{w_2,1,-1} - H_{w_2,-1,0} - H_{w_2,-1,1} + H_{w_2,-1,w_4} + H_{w_2,-1,-1} + H_{w_3,1,w_1} \right.
\end{aligned}$$



$$\begin{aligned}
 & -\mathbb{H}_{w_3,1,w_2} + \mathbb{H}_{w_3,-1,w_1} - \mathbb{H}_{w_3,-1,w_2} + \frac{1}{2} [\ln(k^2 - z^2) - 2 \ln(k^2 - z) + 6 \ln(k) \\
 & - \ln(1 - k^2)] [\mathbb{H}_{w_2,-1} - \mathbb{H}_{w_1,-1} + \mathbb{H}_{w_2,1} - \mathbb{H}_{w_1,1}] + \frac{1}{2} \left( -\mathbb{H}_{w_1,1} - \mathbb{H}_{w_1,-1} + \mathbb{H}_{w_2,1} \right. \\
 & \left. + \mathbb{H}_{w_2,-1} + [\mathbb{H}_{w_1} - \mathbb{H}_{w_2}] \mathbb{H}_1 \right) \mathbb{H}_{-1} + [\mathbb{H}_{w_1,1} + \mathbb{H}_{w_1,-1} - \mathbb{H}_{w_2,1} - \mathbb{H}_{w_2,-1}] \mathbb{H}_{w_3} \\
 & - \frac{1}{2} \left( \mathbb{H}_{1,1} - \mathbb{H}_1^2 + 2\mathbb{H}_{w_3,1} + 2\mathbb{H}_{w_3,-1} + 2\mathbb{H}_{-1,1} + \mathbb{H}_{-1,-1} + k\mathbb{H}_{w_1,1} + k\mathbb{H}_{w_1,-1} \right. \\
 & \left. - k\mathbb{H}_{w_2,1} - k\mathbb{H}_{w_2,-1} \right) [\mathbb{H}_{w_1} - \mathbb{H}_{w_2}] + \frac{1}{2} [\mathbb{H}_{w_1,1} + \mathbb{H}_{w_1,-1} - \mathbb{H}_{w_2,1} - \mathbb{H}_{w_2,-1}] \mathbb{H}_1 \left. \right\} \\
 & - 16k(1 - z^2) \left\{ -\mathbb{H}_{1,w_4,w_5} - \mathbb{H}_{1,w_4,w_6} - \mathbb{H}_{1,w_4,w_7} - \mathbb{H}_{1,w_4,w_8} + \mathbb{H}_{w_5,1,1} - \mathbb{H}_{w_5,1,-1} \right. \\
 & + \mathbb{H}_{w_5,w_3,1} - \mathbb{H}_{w_5,w_3,-1} + \mathbb{H}_{w_6,1,1} - \mathbb{H}_{w_6,1,-1} + \mathbb{H}_{w_6,w_3,1} - \mathbb{H}_{w_6,w_3,-1} + \mathbb{H}_{w_7,w_3,1} \\
 & - \mathbb{H}_{w_7,w_3,-1} - \mathbb{H}_{w_7,-1,1} + \mathbb{H}_{w_7,-1,-1} + \mathbb{H}_{w_8,w_3,1} - \mathbb{H}_{w_8,w_3,-1} - \mathbb{H}_{w_8,-1,1} + \mathbb{H}_{w_8,-1,-1} \\
 & + \mathbb{H}_{-1,w_4,w_5} + \mathbb{H}_{-1,w_4,w_6} + \mathbb{H}_{-1,w_4,w_7} + \mathbb{H}_{-1,w_4,w_8} + k[\mathbb{H}_{w_1,w_4,w_5} + \mathbb{H}_{w_1,w_4,w_6} \\
 & + \mathbb{H}_{w_1,w_4,w_7} + \mathbb{H}_{w_1,w_4,w_8} - \mathbb{H}_{w_2,w_4,w_5} - \mathbb{H}_{w_2,w_4,w_6} - \mathbb{H}_{w_2,w_4,w_7} - \mathbb{H}_{w_2,w_4,w_8} - \mathbb{H}_{w_5,1,w_1} \\
 & + \mathbb{H}_{w_5,1,w_2} - \mathbb{H}_{w_5,w_3,w_1} + \mathbb{H}_{w_5,w_3,w_2} - \mathbb{H}_{w_6,1,w_1} + \mathbb{H}_{w_6,1,w_2} - \mathbb{H}_{w_6,w_3,w_1} + \mathbb{H}_{w_6,w_3,w_2} \\
 & - \mathbb{H}_{w_7,w_3,w_1} + \mathbb{H}_{w_7,w_3,w_2} + \mathbb{H}_{w_7,-1,w_1} - \mathbb{H}_{w_7,-1,w_2} - \mathbb{H}_{w_8,w_3,w_1} + \mathbb{H}_{w_8,w_3,w_2} \\
 & \left. + \mathbb{H}_{w_8,-1,w_1} - \mathbb{H}_{w_8,-1,w_2} \right] + \left( -\mathbb{H}_{1,1} - \mathbb{H}_{w_3,1} + \mathbb{H}_{w_3,-1} - \mathbb{H}_{-1,1} + \mathbb{H}_1^2 - k\mathbb{H}_{w_1,1} \right. \\
 & \left. + k\mathbb{H}_{w_2,1} + k\mathbb{H}_{w_3,w_1} - k\mathbb{H}_{w_3,w_2} \right) [\mathbb{H}_{w_5} + \mathbb{H}_{w_6}] + \left( -\mathbb{H}_{w_3,1} + \mathbb{H}_{w_3,-1} + \mathbb{H}_{-1,1} \right. \\
 & \left. + \mathbb{H}_{-1,-1} - \mathbb{H}_1 \mathbb{H}_{-1} + k\mathbb{H}_{w_1,-1} - k\mathbb{H}_{w_2,-1} + k\mathbb{H}_{w_3,w_1} - k\mathbb{H}_{w_3,w_2} \right) [\mathbb{H}_{w_7} + \mathbb{H}_{w_8}] \\
 & + \left( (\mathbb{H}_{w_5} + \mathbb{H}_{w_6} + \mathbb{H}_{w_7} + \mathbb{H}_{w_8}) \mathbb{H}_{w_3} - \mathbb{H}_{w_5,1} - \mathbb{H}_{w_5,w_3} - \mathbb{H}_{w_6,1} - \mathbb{H}_{w_6,w_3} - \mathbb{H}_{w_7,w_3} \right. \\
 & \left. + \mathbb{H}_{w_7,-1} - \mathbb{H}_{w_8,w_3} + \mathbb{H}_{w_8,-1} \right) \\
 & \times [\mathbb{H}_1 - \mathbb{H}_{-1} - k(\mathbb{H}_{w_1} - \mathbb{H}_{w_2})] \left. \right\} + 576(1 - z)\beta \ln(k) - 96(1 - z)\beta \ln(1 - k^2) \\
 & - 192(1 - z)\beta \mathbb{H}_0 - 192(1 - z)\beta \ln(k^2 - z) \left. \right\} \\
 & + \frac{1}{2} P_{gq}^{(0)} \otimes h_{g_1}^{(1)} L_M - P_{gq}^{(0)} \otimes \bar{b}_{g_1}^{(1)}. \tag{4.46}
 \end{aligned}$$

The remaining convolutions appearing in Eq. (4.46) are given in Appendix D.4. Here the argument of the iterative integrals  $\mathbb{H}_{\vec{a}}$  is  $\beta$ .

The polynomials  $P_i$  in Eq. (4.46) read

$$P_{67} = 3k^4 + 3k^2(z^2 + 1) - z^2, \tag{4.47}$$

$$P_{68} = 6k^4 + 3k^3z(2z - 1) + 6k^2(z^2 - 4z - 1) + 3kz - 2z^2, \tag{4.48}$$

$$P_{69} = 6k^4 + 3k^3(2z^2 - 5z + 8) + 6k^2(z^2 + 2z + 2) + 3kz - 2z^2, \tag{4.49}$$

$$P_{70} = 6k^4z + k^3(-16z^3 + 33z^2 - 24z + 8) + 6k^2z(z^2 + 2z + 2) - 3kz^2 - 2z^3, \tag{4.50}$$

$$P_{71} = 6k^4z + k^3(-4z^3 + 3z^2 + 24z + 8) + 6k^2z(z^2 + 2z + 2) + 3kz^2 - 2z^3, \tag{4.51}$$

$$P_{72} = 6k^4z + k^3(4z^3 - 3z^2 - 24z - 8) + 6k^2z(z^2 + 2z + 2) - 3kz^2 - 2z^3, \tag{4.52}$$

$$P_{73} = 6k^4z + k^3(16z^3 - 33z^2 + 24z - 8) + 6k^2z(z^2 + 2z + 2) + 3kz^2 - 2z^3, \tag{4.53}$$

#### 4. Polarized Pure-Singlet Wilson Coefficients at NLO

$$P_{74} = 3\beta k^3(z-3) + 3k^2(z-4) + 4\beta k(3z^2 - 13z + 3) - 12z^2 + 46z + 9, \quad (4.54)$$

$$P_{75} = 3\beta k^3(z-3) - 3k^2(z-4) + 4\beta k(3z^2 - 13z + 3) + 12z^2 - 46z - 9, \quad (4.55)$$

$$P_{76} = 3\beta k^4(1-z)^2 + k^3(-35\beta + (3-16\beta)z^2 + 3(17\beta-9)z + 39) + k^2(-52\beta + 12\beta z^3 + (22-81\beta)z^2 + (121\beta-72)z + 35) + k(12(\beta-1)z^3 + (75-38\beta)z^2 + (26\beta-88)z + 10) + z(-12z^2 + 32z - 5), \quad (4.56)$$

$$P_{77} = 3\beta k^4(1-z)^2 + k^3(35\beta + (16\beta-3)z^2 + (27-51\beta)z - 39) + k^2(-52\beta + 12\beta z^3 + (22-81\beta)z^2 + (121\beta-72)z + 35) + k(-12(\beta-1)z^3 + (38\beta-75)z^2 + (88-26\beta)z - 10) + z(-12z^2 + 32z - 5), \quad (4.57)$$

$$P_{78} = 3\beta k^4(1-z)^2 - k^3(35\beta + (16\beta+3)z^2 - 3(17\beta+9)z + 39) + k^2(-52\beta + 12\beta z^3 - (81\beta+22)z^2 + (121\beta+72)z - 35) + k(12(\beta+1)z^3 - (38\beta+75)z^2 + (26\beta+88)z - 10) + z(12z^2 - 32z + 5), \quad (4.58)$$

$$P_{79} = 3\beta k^4(1-z)^2 + k^3(35\beta + (16\beta+3)z^2 - 3(17\beta+9)z + 39) + k^2(-52\beta + 12\beta z^3 - (81\beta+22)z^2 + (121\beta+72)z - 35) + k(-12(\beta+1)z^3 + (38\beta+75)z^2 - 2(13\beta+44)z + 10) + z(12z^2 - 32z + 5), \quad (4.59)$$

$$P_{80} = k^4(-3(36\beta+1) + (27\beta-10)z^3 + (37-135\beta)z^2 + (216\beta-34)z) + k^2z((3-27\beta)z^2 + (27\beta+28)z - 28) + 7z^3, \quad (4.60)$$

$$P_{81} = k^4(-108\beta + (27\beta+10)z^3 - (135\beta+37)z^2 + (216\beta+34)z + 3) + k^2z(-3(9\beta+1)z^2 + (27\beta-28)z + 28) - 7z^3. \quad (4.61)$$

#### 4.4. The Asymptotic and Threshold Expansions

The complete expressions calculated in Section 4.3 allow now to perform the asymptotic expansion for  $Q^2 \gg m^2$  and the threshold expansion for  $\beta \ll 1$ .

In the asymptotic limit  $Q^2 \gg m^2$  and setting  $\mu^2 = Q^2$  the first expansion coefficients of the polarized massive pure singlet Wilson coefficient read

$$\begin{aligned} H_{g_1}^{(2),\text{PS},L} &= C_F T_F \left\{ -(20(1-z) + 8(1+z)H_0) \ln^2\left(\frac{m^2}{Q^2}\right) - (8(1-z) - 8(1-3z)H_0 \right. \\ &\quad - 8(1+z)H_0^2) \ln\left(\frac{m^2}{Q^2}\right) + \frac{592}{3}(1-z) + \left(\frac{256}{3}(2-z) - \frac{32(1+z)^3}{3z}H_{-1}\right)H_0 \\ &\quad + \frac{8}{3}(21+2z^2)H_0^2 + \frac{16}{3}(1+z)H_0^3 + \left(88(1-z) + 80(1-z)H_0\right)H_1 + 20(1-z)H_1^2 \\ &\quad - \left(16(1-3z) - 32(1+z)H_0\right)H_{0,1} + \frac{32(1+z)^3}{3z}H_{0,-1} - 32(1+z)H_{0,0,1} \\ &\quad + 16(1+z)H_{0,1,1} - \left(\frac{32}{3}(9-3z+z^2) + 32(1+z)H_0\right)\zeta_2 + 16(1+z)\zeta_3 \\ &\quad + \frac{m^2}{Q^2} \left[ (16(1-z)(1-3z) - 32zH_0) \ln\left(\frac{m^2}{Q^2}\right) + 8(18-12z-7z^2) \right. \\ &\quad \left. + 16(6+z+6z^2)H_0 + 16zH_0^2 + 16(3-7z+3z^2)H_1 \right] \\ &\quad + \left(\frac{m^2}{Q^2}\right)^2 \left[ -4(1-z)(3+4z) \ln^2\left(\frac{m^2}{Q^2}\right) + \left(\frac{4P_{84}}{1-z} - 16(1-z)(5+4z)H_0 \right. \right. \end{aligned}$$

$$\begin{aligned}
 & -8(1-z)(5+4z)H_1 \Big) \ln\left(\frac{m^2}{Q^2}\right) + \frac{2P_{85}}{3(1-z)^2} + \left(\frac{16P_{82}}{1-z} - 64(1-z^2)H_{-1}\right)H_0 \\
 & + \left(\frac{4P_{83}}{1-z} - 32(1-z)H_0\right)H_1 - 4(1-z)(7+4z)H_1^2 - 16(1-z)(3+4z)H_{0,1} \\
 & + 64(1-z^2)H_{0,-1} + 16(1-z)\zeta_2 \Big] + O(\kappa^3 \ln^2(\kappa)) \Big\}, \tag{4.62}
 \end{aligned}$$

with  $\kappa = m^2/Q^2$  and the polynomials

$$P_{82} = 3z^4 + z^3 - 11z^2 + 13z - 7, \tag{4.63}$$

$$P_{83} = 6z^4 + 2z^3 - 63z^2 + 84z - 32, \tag{4.64}$$

$$P_{84} = 6z^4 + 2z^3 - 57z^2 + 76z - 28, \tag{4.65}$$

$$P_{85} = 15z^5 - 27z^4 + 393z^3 - 1079z^2 + 1069z - 339. \tag{4.66}$$

In this expansion the Kummer-elliptic integrals turn into harmonic polylogarithms. The leading term, which is free of power corrections of  $\mathcal{O}((m^2/Q^2)^k)$ ,  $k \in \mathbb{N}$ ,  $k \geq 1$ , can be predicted using the representation of the massive Wilson coefficient by massive operator matrix elements (OMEs), cf. [173, 179, 185, 302], and massless Wilson coefficients,

$$H_{g_1}^{(2),\text{PS},L}\left(z, \frac{Q^2}{m^2}\right) = A_{Qq}^{(2),\text{PS}}(N_F + 1) + \tilde{C}_{g_1}^{(2),\text{PS},L}(N_F + 1). \tag{4.67}$$

Here the massless Wilson coefficient  $\tilde{C}_{g_1}^{(2),\text{PS}}(N_F + 1)$  is the one given in Eq. (4.35) normalized by  $N_F + 1$ . The massive two-loop operator matrix element  $A_{Qq}^{(2),\text{PS}}$  in Mellin space reads

$$A_{Qq}^{(2),\text{PS}} = -\frac{1}{8}\hat{P}_{qg}^{(0)}P_{gq}^{(0)}\ln^2\left(\frac{m^2}{\mu^2}\right) - \frac{1}{2}\hat{P}_{qg}^{(1),\text{PS}}\ln\left(\frac{m^2}{\mu^2}\right) + \frac{1}{8}\hat{P}_{qg}^{(0)}P_{gq}^{(0)}\zeta_2 + a_{Qq}^{(2),\text{PS}}, \tag{4.68}$$

cf. [173, 179, 185, 302]; for its renormalization see Ref. [182]. The constant part of the unrenormalized polarized OME  $a_{Qq}^{(2),\text{PS}}$  is given by [173, 302]

$$\begin{aligned}
 a_{Qq}^{(2),\text{PS}}(z) = & C_F T_F \Big\{ -72(1-z) - 12(1+5z)H_0 - 2(1-3z)H_0^2 - \frac{4}{3}(1+z)H_0^3 + 40(1-z)H_0H_1 \\
 & - (40(1-z) - 16(1+z)H_0)H_{0,1} - 32(1+z)H_{0,0,1} - (20(1-z) - 8(1+z)H_0)\zeta_2 \\
 & + 32(1+z)\zeta_3 \Big\} \tag{4.69}
 \end{aligned}$$

in  $z$ -space. The calculation of  $A_{Qq}^{(2),\text{PS}}$  is performed in the Larin scheme. One has either to apply the tensor decomposition method or use the new projector introduced in Chapter 8, however, to obtain the correct result. These aspects are discussed in Chapter 8 and Ref. [302] in detail. The asymptotic result is correctly reproduced.

The threshold expansion of the Wilson coefficients for  $\beta \ll 1$  is given by

$$\begin{aligned}
 H_{g_1}^{(1)}\left(z, \frac{Q^2}{m^2}\right) = & 4T_F\beta \Big\{ 1 - \frac{2}{3}(1-2z)\beta^2 - \frac{2}{5}(1-2z)\beta^4 - \frac{2}{7}(1-2z)\beta^6 \\
 & - \frac{2}{9}(1-2z)\beta^8 + \mathcal{O}(\beta^{10}) \Big\}, \tag{4.70}
 \end{aligned}$$

$$H_{g_1}^{(2),\text{PS},L}\left(z, \frac{Q^2}{m^2}\right) = C_F T_F (1-z)\beta^3 \Big\{ -\frac{256}{9} + \frac{16}{3}[\ln(1-z) - \ln(z) + 4\ln(2\beta)] \Big\} \tag{4.71}$$

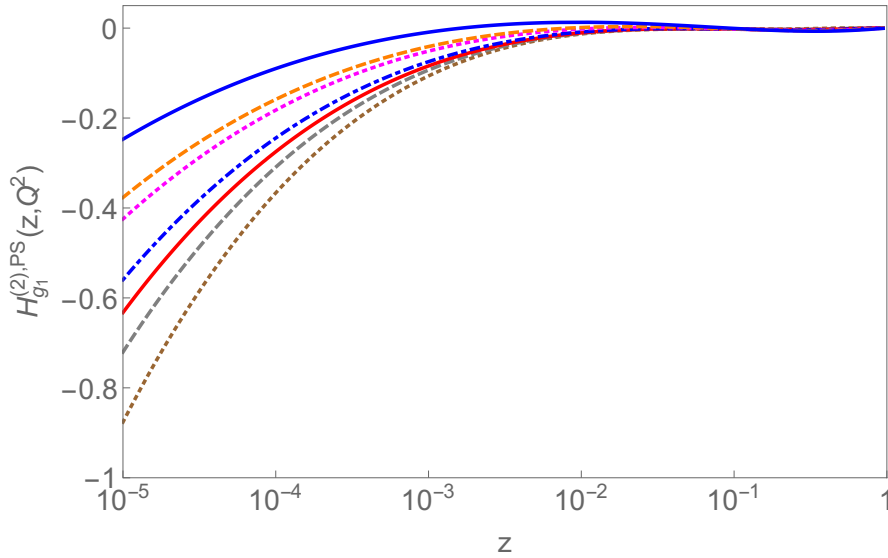


Figure 4.1.: The Wilson coefficient  $H_{g_1}^{(2),\text{PS}}$  as a function of  $z$  for different values of  $Q^2$  and the scale choice  $\mu^2 = \mu_F^2 = Q^2$ . Upper full line (Blue):  $Q^2 = 10\,000\text{ GeV}^2$ ; upper dashed line (Orange):  $Q^2 = 1000\text{ GeV}^2$ ; upper dotted line (Magenta):  $Q^2 = 500\text{ GeV}^2$ ; dash-dotted line (Blue):  $Q^2 = 100\text{ GeV}^2$ ; lower full line (Red):  $Q^2 = 50\text{ GeV}^2$ ; lower dashed line (Gray):  $Q^2 = 25\text{ GeV}^2$ ; lower dotted line (Brown):  $Q^2 = 10\text{ GeV}^2$ .

$$\begin{aligned}
 & +\beta^2 \left( -\frac{32}{75}(41 + 20z) + \frac{16}{5} [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] \right) \\
 & -\beta^4 \left( \frac{16(2723 + 20504z - 12352z^2)}{11025} - \frac{16}{105} (7 + 16z - 8z^2) [\ln(1-z) \right. \\
 & \left. - \ln(z) + 4 \ln(2\beta)] \right) + \beta^6 \left( \frac{16(47203 - 909904z + 950864z^2 - 345728z^3)}{297675} \right. \\
 & \left. + \frac{16}{945} (1 + 272z - 232z^2 + 64z^3) [\ln(1-z) - \ln(z) + 4 \ln(2\beta)] \right) \\
 & \left. + \mathcal{O}(\beta^8) \right\}.
 \end{aligned}$$

## 4.5. Numerical Results

Let us now illustrate the analytic results numerically. In Fig. 4.1 the two-loop heavy flavor Wilson coefficient  $H_{g_1}^{(2),\text{PS},L}$  is shown as a function of  $z$  for different values of  $Q^2 \in [10, 10^4]\text{ GeV}^2$ . We work in the on-shell scheme and therefore set the charm quark mass to its pole mass,  $m_c = 1.59\text{ GeV}$ , cf. [256]. For large values of  $Q^2$  these results approach the asymptotic result for  $H_{g_1}^{(2),\text{PS}}$ . In the small  $x$  region this Wilson coefficient is negative.

Next we study the ratios

$$R_{g_1}^{(1)} = \frac{H_{g_1}^{(2),\text{PS}}}{\tilde{H}_{g_1}^{(2),\text{PS}}}(\mu = \mu_F = m), \quad (4.72)$$

comparing the full, cf. Eq. (4.46) and the asymptotic results,  $\tilde{H}$ , Eq. (4.62) for the leading term in Fig. 4.2.

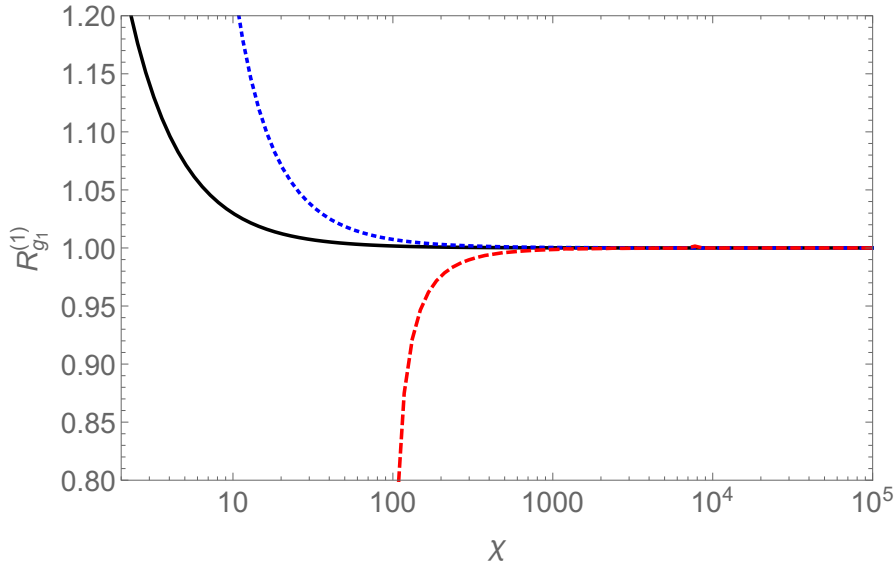


Figure 4.2.: The ratio  $R_{g_1}^{(1)}$ , Eq. (4.72), as a function of  $\chi = Q^2/m^2$ . Solid line:  $z = 10^{-4}$ ; dotted line:  $z = 10^{-2}$ ; dashed line:  $z = 1/2$ .

For  $H_{g_1}^{(2),\text{PS}}$  the asymptotic expansion agrees with the full calculation up to  $Q^2/m^2 \equiv \chi = 10$  to about 2% for  $z = 10^{-4}$ ,  $\chi = 40$  for  $z = 10^{-2}$  and  $\chi = 200$  for  $z = 1/2$ . However, the Wilson coefficients are very small already for the last value. Similar to the ratio of the full and asymptotic Wilson coefficient we define the ratio

$$R_{g_1} = \frac{g_1^{(2),\text{PS}}}{\tilde{g}_1^{(2),\text{PS}}}, \quad (4.73)$$

where  $\tilde{g}_1^{(2),\text{PS}}$  is the structure function obtained by using the expansion of the respective Wilson coefficient up to the desired level. The corresponding results are depicted in Fig. 4.3. We use the parameterization of the parton distributions Ref. [320] at NLO with the corresponding values of  $\alpha_s(Q^2)$  at NNLO [207] to compare to previous non-singlet results in [305]. Demanding an agreement within  $\pm 2\%$  for  $g_1^{\text{PS}}$  in the range  $z \in [10^{-4}, 10^{-2}, 1/2]$  leads to values  $Q_0^2/m^2 \in [5, 5, 13]$  of the  $\mathcal{O}((m^2/Q^2)^2)$  improved result,  $Q_0^2/m^2 \in [10, 12, 30]$  of the  $\mathcal{O}(m^2/Q^2)$  improved result, and  $Q_0^2/m^2 \in [12, 100, 170]$  for the asymptotic result.

In Figures 4.4 we show the complete results for the two-loop pure singlet contributions to  $xg_1$  and  $xg_2$  as a function of  $x$  for a series of  $Q^2$ -values. Both functions show an oscillatory behavior, which is enlarged for  $xg_2$  due to the Wandzura–Wilczek relation, cf. Eq. (4.10) [162]. In Fig. 4.5 we illustrate the ratios Eq. (4.73) as a function of  $x$  for different values of  $Q^2$  for  $g_1^{\text{PS}}$  comparing the asymptotic result to the full result. For a better visibility and to avoid to depict zero transitions in the denominator we separate the small  $x$  and large  $x$  part into two figures. The corrections behave widely flat in  $x$  for larger values of  $Q^2$  and develop some profile for  $Q^2 < 100 \text{ GeV}^2$ .

In Fig. 4.6 we depict the ratio of the full result over the  $\mathcal{O}((m^2/Q^2)^2)$  improved asymptotic results for  $g_1^{\text{PS}}$  as a function of  $x$  for a series of  $Q^2$ -values, again separating the small  $x$  and the large  $x$  ranges because of zero transitions for this ratio. For  $Q^2 \gtrsim 100 \text{ GeV}^2$  the ratios are rather flat and are close to one. The line for  $Q^2 = 100 \text{ GeV}^2$  for  $x > 0.5$  deviates from one by more than 5%. Larger deviations are found for  $Q^2 = 50 \text{ GeV}^2$ , where the 5% margin is only met for  $x < 3 \cdot 10^{-3}$ . As in the unpolarized case, we limited the expansion to terms of  $\sim \mathcal{O}((m^2/Q^2)^2)$ , but higher order terms can be given straightforwardly. The expanded expressions do also allow direct Mellin transforms and provide a suitable analytic basis for Mellin-space programmes.

#### 4. Polarized Pure-Singlet Wilson Coefficients at NLO

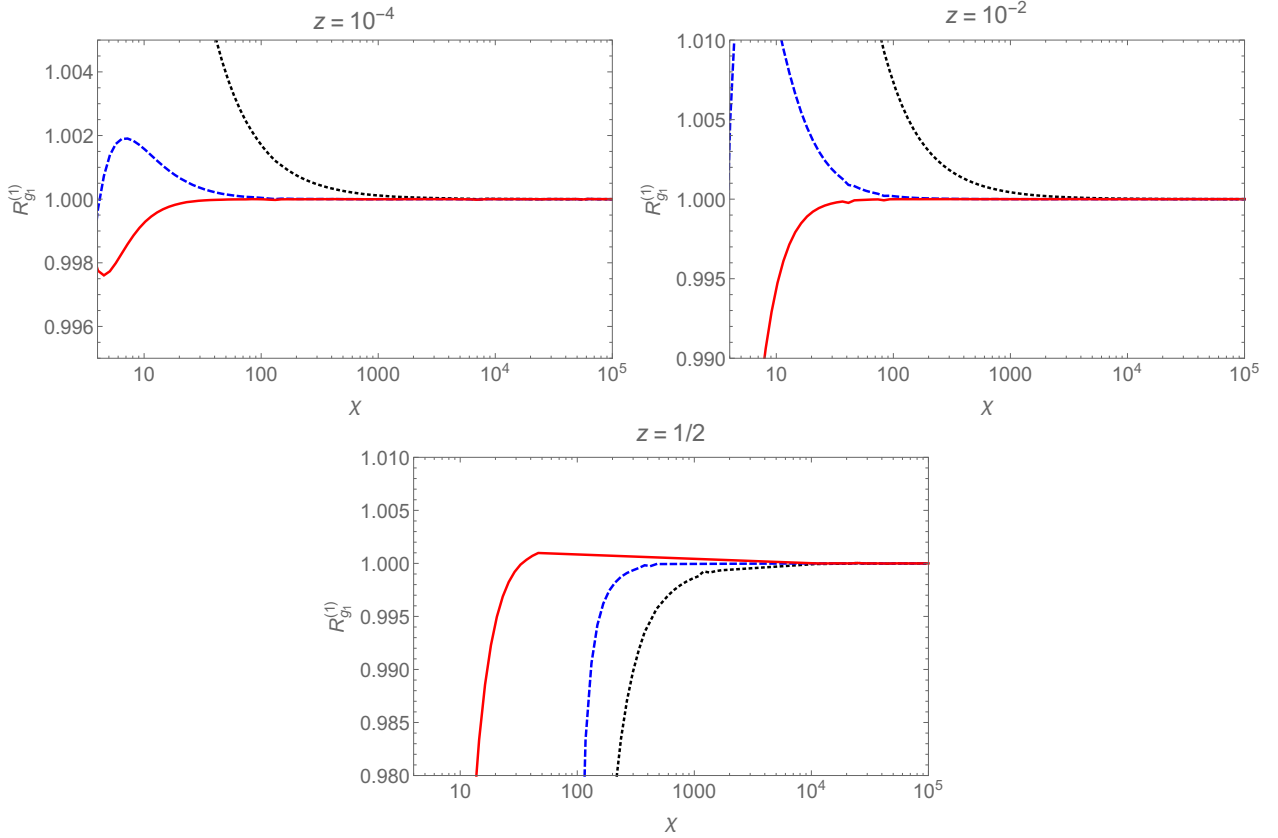


Figure 4.3.: The ratio  $R_{g_1}^{(1)}$ , Eq. (4.72), as a function of  $\chi = Q^2/m^2$  for different values of  $z$  gradually improved with  $\kappa$  suppressed terms. Dotted lines: asymptotic result; dashed lines:  $\mathcal{O}(m^2/Q^2)$  improved; solid lines :  $\mathcal{O}((m^2/Q^2)^2)$  improved.

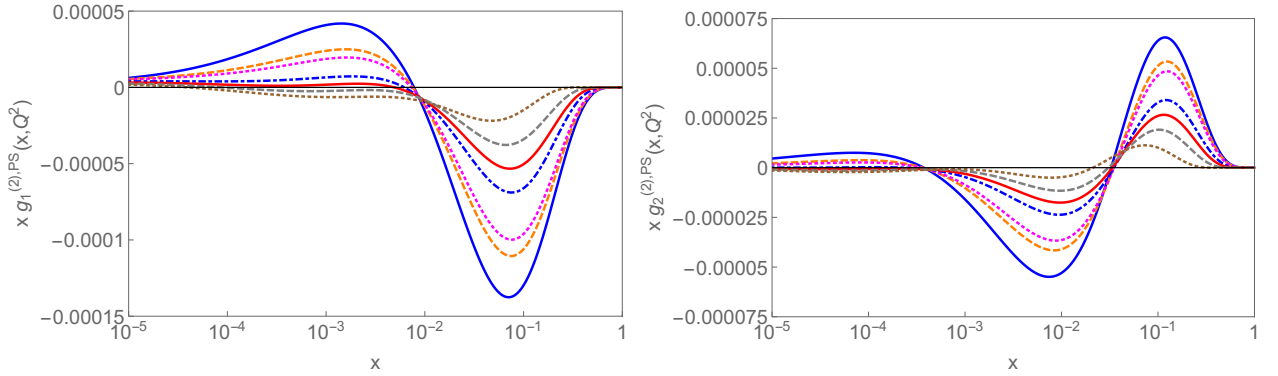


Figure 4.4.: The pure singlet contributions  $xg_1^{(2),\text{PS}}$  and  $xg_2^{(2),\text{PS}}$  for different values of  $Q^2$  and the scale choice  $\mu^2 = \mu_F^2 = Q^2$ . Full line (Blue):  $Q^2 = 10\,000\text{ GeV}^2$ ; dashed line (Orange):  $Q^2 = 1000\text{ GeV}^2$ ; dotted line (Magenta):  $Q^2 = 500\text{ GeV}^2$ ; dash-dotted line (Blue):  $Q^2 = 100\text{ GeV}^2$ ; full line (Red):  $Q^2 = 50\text{ GeV}^2$ ; dashed line (Gray):  $Q^2 = 25\text{ GeV}^2$ ; dotted line (Brown):  $Q^2 = 10\text{ GeV}^2$ , using the parameterization of the parton distribution [320].

To summarize, we have calculated the massless and massive polarized two-loop pure singlet Wilson coefficients for deep-inelastic scattering in analytic form. The calculation has been performed in the Larin scheme, with a final finite renormalization to the  $M$ -scheme in the massless case. The finite renormalization in the massless case has been derived in Refs. [152]. The massless Wilson coefficient

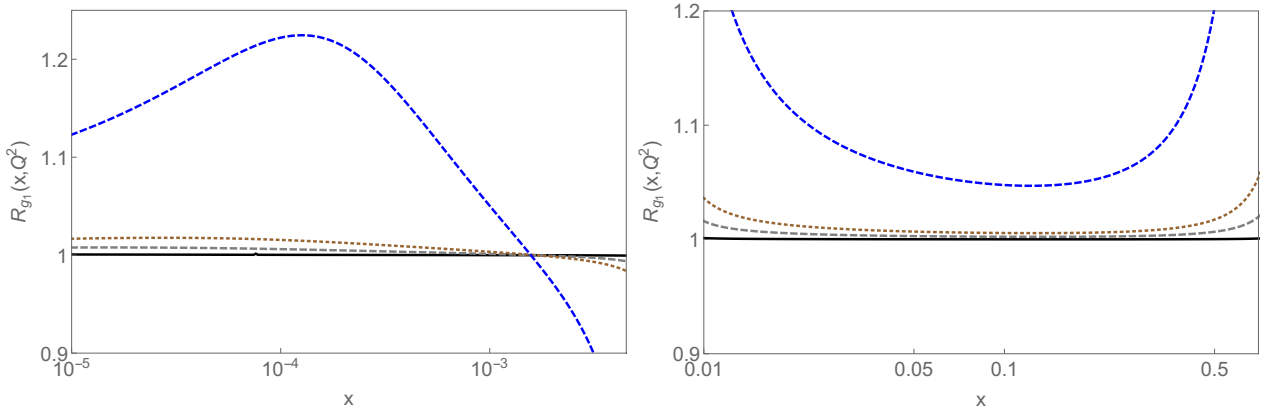


Figure 4.5.: The ratio of the structure function  $g_1^{(2),\text{PS}}$  in the full calculation over the asymptotic approximation for different values of  $Q^2$  and the scale choice  $\mu^2 = \mu_F^2 = Q^2$ . Full line (Black):  $Q^2 = 10\,000\text{ GeV}^2$ ; dashed line (Gray):  $Q^2 = 1000\text{ GeV}^2$ ; dotted line (Brown):  $Q^2 = 500\text{ GeV}^2$ ; lower dashed line (Blue):  $Q^2 = 100\text{ GeV}^2$ , using the parameterization of the parton distribution [320]

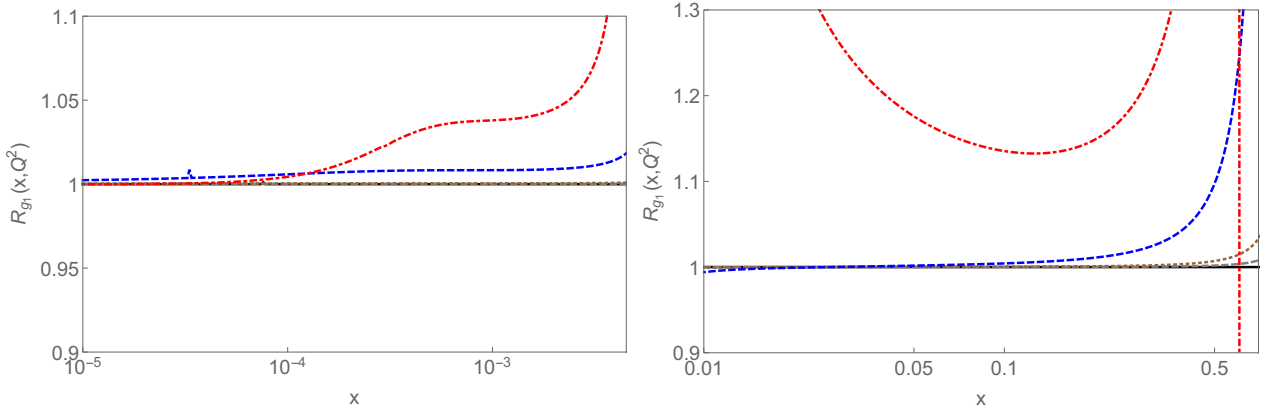


Figure 4.6.: The ratio of the pure singlet structure function  $g_1^{(2),\text{PS}}$  in the full calculation over the  $\mathcal{O}((m^2/Q^2)^2)$  improved approximation for different values of  $Q^2$  and the scale choice  $\mu^2 = \mu_F^2 = Q^2$ . Full lines (Black):  $Q^2 = 10\,000\text{ GeV}^2$ ; dashed lines (Gray):  $Q^2 = 1000\text{ GeV}^2$ ; dotted lines (Brown):  $Q^2 = 500\text{ GeV}^2$ ; dashed lines (Blue):  $Q^2 = 100\text{ GeV}^2$ ; dash-dotted lines (Red):  $Q^2 = 50\text{ GeV}^2$ , using the parameterization of the parton distribution [320].

can be expressed by the harmonic polylogarithms in  $z$ -space and harmonic sums in Mellin- $N$  space. In the massive case the polarized two-loop pure singlet Wilson coefficient is also given by iterative integrals, however, of a more general kind, the Kummer-elliptic integrals, here based on an alphabet of 12 letters, cf. [5]. From the expansion of the massive Wilson coefficient in the region  $Q^2 \gg m^2$  one obtains the asymptotic result, which can be given in terms of a massive OME and the massless Wilson coefficient, cf. [302]. In the region of lower values of  $Q^2$  and larger values of  $x$ , the power corrections to the massive two-loop Wilson coefficient are essential. From the available analytic result one can construct the series in  $m^2/Q^2$  analytically. Since the deep-inelastic process is usually considered only for virtualities  $Q^2 \gtrsim 5\text{ GeV}^2$ , this series gives the proper numerical representation in case of the charm-quark corrections retaining a relatively small number of terms. The latter representation has the advantage that it can be transformed into Mellin space directly, since the expansion coefficients are given in terms of harmonic polylogarithms in  $z$ -space.





## 5. Renormalization of the Massive Operator Matrix Elements in the Two-Mass Case

The renormalization of the operator matrix elements for deep-inelastic scattering up to  $\mathcal{O}(a_s^3)$  has been carried out in the single mass case in [182] and in the two mass case in [202]. During the calculations presented in the next chapters it, however, became clear that one should use a more consistent notation in the two mass case. Furthermore some steps of the renormalization were only given in an power expansion in  $\eta$  since the full analytic results have not yet been available. We will therefore address these aspects once again. The presentation will, however, closely follow the original work [182, 202].

The Feynman integrals contributing to the various operator matrix elements contain mass, coupling, ultraviolet operator singularities, and collinear divergences, due to massless sub-graphs. They are regularized by applying dimensional regularization [56] in  $d = 4 + \varepsilon$  dimensions. The singularities appear as poles in the Laurent series in  $\varepsilon$ , with the highest pole corresponding to the loop order. At one and two loop order the two-mass massive operator matrix elements  $\tilde{A}_{ij}$  are given in terms of the known single mass contributions since they do not contain more than one internal massive fermion line [179, 180, 184–187, 254, 260].

The first single particle irreducible diagrams with two masses emerge at  $\mathcal{O}(\alpha_s^3)$ . In the following, we consider the renormalization of the two mass contributions in individual terms together with the genuine two-mass contributions. The latter terms will then be obtained subtracting the former ones, cf. Ref. [182]. The unrenormalized OMEs are given by

$$\hat{A}_{ij}^{(l)}\left(\frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) = \hat{A}_{ij}^{(l)}\left(\frac{m_1^2}{\mu^2}\right) + \hat{A}_{ij}^{(l)}\left(\frac{m_2^2}{\mu^2}\right) + \hat{\hat{A}}_{ij}^{(l)}\left(\frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right), \quad (5.1)$$

where  $\hat{A}_{ij}^{(l)}\left(\frac{m_1^2}{\mu^2}\right)$  are the single-mass OMEs [182] and  $\hat{\hat{A}}_{ij}^{(l)}$  are the two-mass contributions. A change in the renormalization scheme as in Eqs. (5.39) and (5.40) generally introduces a mixing between the different components of Eq. (5.1). Here we introduced the two masses  $m_1$  and  $m_2$ . We set  $m_2 < m_1$  so that

$$\eta = \frac{m_2^2}{m_1^2} < 1. \quad (5.2)$$

In the following we will also need the logarithms

$$L_1 = \ln\left(\frac{m_1^2}{\mu^2}\right), \quad L_2 = \ln\left(\frac{m_2^2}{\mu^2}\right), \quad L_\eta = \ln(\eta) \quad (5.3)$$

where  $\mu$  is the renormalization scale.

The renormalization procedure follows the one outlined in Ref. [182], incorporating the necessary modifications for the two-mass case. Here the case of  $N_F$  massless and two massive quark flavors is considered as this covers the physical case of contributions due to the charm and bottom quarks. The large mass gap to the top quark in general allows to decouple it after the charm and the bottom quark and thus does not have to be included into a scheme with  $N_F$  massless and three massive quarks. Since in this chapter again two massive quarks are considered we will use the notation

$$\tilde{f}(x) = \frac{f(x)}{x}, \quad (5.4)$$

$$\hat{f}(x) = f(x+2) - f(x) \quad (5.5)$$

to abbreviate certain expressions. Note that these notations never apply to OMEs but only to anomalous dimensions  $\gamma_{ij}$  in this section. The differences with respect to [202] mainly lie in the use of Eq. (5.5) instead of the convention with one heavy quark. Furthermore the notation  $\hat{f}(x)$  was used to represent the coefficient of the  $N_F^2$  dependent term of certain anomalous dimensions. However this is not in accordance with the conventions for anomalous dimensions which start with  $N_F^0$ . These terms will be denoted by  $f^{N_F^2}$  in the following. Also the inclusion of reducible contributions introduces some subtleties for OMEs with external gluons. This issue will be further clarified in Section 5.5.

In the following sections first the mass and coupling constant renormalization is considered, followed by the renormalization of the ultraviolet singularity of the local operators, and the factorization of the collinear singularities.

## 5.1. Mass Renormalization

The schemes most frequently used for the mass renormalization are the  $\overline{\text{MS}}$ - and the on-mass shell scheme (OMS). In the following, the mass is renormalized in the OMS and the finite renormalization to switch to the  $\overline{\text{MS}}$ -mass is provided at a later stage. The mass renormalization is applied first, i.e. the respective expressions are still containing the bare coupling  $\hat{a}_s = \hat{g}_s^2/(4\pi)^2$ .<sup>1</sup>

The bare masses  $\hat{m}_i$ ,  $i \in \{1, 2\}$  are expressed by the renormalized on-shell masses  $m_i$  via

$$\hat{m}_i = Z_{m,i}(m_1, m_2) m_i = m_i \left[ 1 + \hat{a}_s \left( \frac{m_i^2}{\mu^2} \right)^{\varepsilon/2} \delta m_1 + \hat{a}_s^2 \left( \frac{m_i^2}{\mu^2} \right)^{\varepsilon} \delta m_{2,i}(m_1, m_2) \right] + \mathcal{O}(\hat{a}_s^3), \quad (5.6)$$

and

$$\delta m_{2,i}(m_1, m_2) = \delta m_2^0 + \tilde{\delta} m_2^i(m_1, m_2). \quad (5.7)$$

Here  $\delta m_2^0$  is the single mass-contribution, whereas  $\tilde{\delta} m_2^i$  denotes the additional contribution emerging in the case of two massive flavors. Note that from order  $\mathcal{O}(\hat{a}_s^2)$  onward the  $Z$ -factor renormalizing  $\hat{m}_1$  depends on  $m_2$  and vice versa. For the massive operator matrix elements this can be observed at 3-loop order for the first time. The coefficients  $\delta m_1$  and  $\delta m_2$  have been derived in [325, 326] up to  $\mathcal{O}(\varepsilon^0)$  and  $\mathcal{O}(\varepsilon^{-1})$ , respectively. The constant part of  $\delta m_2$  was given in [321, 327, 328] and the  $\mathcal{O}(\varepsilon)$ -term of  $\delta m_1$  in [182]. One obtains

$$\delta m_1 = C_F \left[ \frac{6}{\varepsilon} - 4 + \left( 4 + \frac{3}{4} \zeta_2 \right) \varepsilon \right] \quad (5.8)$$

$$\equiv \frac{\delta m_1^{(-1)}}{\varepsilon} + \delta m_1^{(0)} + \delta m_1^{(1)} \varepsilon, \quad (5.9)$$

$$\begin{aligned} \delta m_2^0 = & C_F \left[ \frac{1}{\varepsilon^2} (18C_F - 22C_A + 8T_F(N_F + 1)) + \frac{1}{\varepsilon} \left( -\frac{45}{2}C_F + \frac{91}{2}C_A \right. \right. \\ & \left. \left. - 14T_F(N_F + 1) \right) + C_F \left( \frac{199}{8} - \frac{51}{2}\zeta_2 + 48 \ln(2)\zeta_2 - 12\zeta_3 \right) + C_A \left( -\frac{605}{8} \right. \right. \\ & \left. \left. + \frac{5}{2}\zeta_2 - 24 \ln(2)\zeta_2 + 6\zeta_3 \right) + T_F \left[ N_F \left( \frac{45}{2} + 10\zeta_2 \right) + \frac{69}{2} - 14\zeta_2 \right] \right] \quad (5.10) \end{aligned}$$

$$\equiv \frac{\delta m_2^{0,(-2)}}{\varepsilon^2} + \frac{\delta m_2^{0,(-1)}}{\varepsilon} + \delta m_2^{0,(0)}, \quad (5.11)$$

<sup>1</sup>Note that this notation therefore agrees with [321], but e.g. differs from the notation in [322–324], where also the charge renormalization has been carried out.

$$\begin{aligned} \tilde{\delta}m_2^i(m_1, m_2) &= C_F T_F \left\{ \frac{8}{\varepsilon^2} - \frac{14}{\varepsilon} + 8r_i^4 H_0^2(r_i) - 8(r_i + 1)^2 (r_i^2 - r_i + 1) H_{-1,0}(r_i) \right. \\ &\quad + 8(r_i - 1)^2 (r_i^2 + r_i + 1) H_{1,0}(r_i) + 8r_i^2 H_0(r_i) + \frac{3}{2} (8r_i^2 + 15) \\ &\quad \left. + 2 \left[ 4r_i^4 - 12r_i^3 - 12r_i + 5 \right] \zeta_2 \right\} \end{aligned} \quad (5.12)$$

$$\equiv \frac{\tilde{\delta}m_2^{(-2)}}{\varepsilon^2} + \frac{\tilde{\delta}m_2^{(-1)}}{\varepsilon} + \tilde{\delta}m_2^{i,(0)}, \quad (5.13)$$

cf. Ref. [321],  $i \in \{1, 2\}$  and

$$r_1 = \sqrt{\eta} \quad \text{and} \quad r_2 = \frac{1}{\sqrt{\eta}}. \quad (5.14)$$

The superscript  $i$  for the coefficients  $\tilde{\delta}m_2^{(-2)}$  and  $\tilde{\delta}m_2^{(-1)}$  has been dropped as they are independent of the renormalized mass  $m_i$ . The harmonic polylogarithms used to express the result in Eq. (5.12) are defined in Appendix C.4.

Applying Eq. (5.6) we obtain the mass renormalized operator matrix elements by

$$\begin{aligned} \hat{A}_{ij} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) &= \delta_{ij} + \hat{a}_s \hat{A}_{ij}^{(1)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) + \hat{a}_s^2 \left\{ \hat{A}_{ij}^{(2)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) \right. \\ &\quad \left. + \delta m_1 \left[ \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} m_1 \frac{d}{dm_1} + \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} m_2 \frac{d}{dm_2} \right] \hat{A}_{ij}^{(1)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) \right\} \\ &\quad + \hat{a}_s^3 \left\{ \hat{A}_{ij}^{(3)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) \right. \\ &\quad + \delta m_1 \left[ \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} m_1 \frac{d}{dm_1} + \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} m_2 \frac{d}{dm_2} \right] \hat{A}_{ij}^{(2)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) \\ &\quad + \delta m_{2,1}(m_1, m_2) \left( \frac{m_1^2}{\mu^2} \right)^\varepsilon m_1 \frac{d}{dm_1} \hat{A}_{ij}^{(1)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) \\ &\quad + \delta m_{2,2}(m_1, m_2) \left( \frac{m_2^2}{\mu^2} \right)^\varepsilon m_2 \frac{d}{dm_2} \hat{A}_{ij}^{(1)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) \\ &\quad + \frac{(\delta m_1)^2}{2} \left[ \left( \frac{m_1^2}{\mu^2} \right)^\varepsilon m_1^2 \frac{d^2}{dm_1^2} + \left( \frac{m_2^2}{\mu^2} \right)^\varepsilon m_2^2 \frac{d^2}{dm_2^2} \right] \hat{A}_{ij}^{(1)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) \\ &\quad \left. + (\delta m_1)^2 \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} m_1 \frac{d}{dm_1} m_2 \frac{d}{dm_2} \hat{A}_{ij}^{(1)} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, \varepsilon, N \right) \right\}, \end{aligned} \quad (5.15)$$

which generalizes Eq. (3.10) of Ref. [182]. The OMEs are symmetric under the interchange of the masses  $m_1$  and  $m_2$ .

## 5.2. Renormalization of the Coupling

When renormalizing the coupling constant, it is important to note that the factorization relation in Eqs. (2.93-2.97) strictly requires the external massless partonic legs of the operator matrix elements to be on-shell, i.e.

$$p^2 = 0, \quad (5.16)$$

## 5. Renormalization of the Massive Operator Matrix Elements in the Two-Mass Case

with  $p$  the external momentum of the OME. This condition would be violated by naively applying massive loop corrections to the gluon propagator. Following [182] it is possible to absorb these corrections uniquely into the coupling constant by using the background field method [329–331] to maintain the Slavnov-Taylor identities of QCD. In this way, one first obtains the coupling constant in a MOM-scheme. A finite renormalization to transform to the  $\overline{\text{MS}}$ -scheme is applied subsequently.

The light flavor contributions to the unrenormalized coupling constant in terms of the renormalized coupling constant in the  $\overline{\text{MS}}$ -scheme read

$$\begin{aligned}\hat{a}_s &= Z_g^{\overline{\text{MS}}}(\varepsilon, N_F) a_s^{\overline{\text{MS}}}(\mu^2) \\ &= a_s^{\overline{\text{MS}}}(\mu^2) \left[ 1 + \delta a_{s,1}^{\overline{\text{MS}}}(N_F) a_s^{\overline{\text{MS}}}(\mu^2) + \delta a_{s,2}^{\overline{\text{MS}}}(N_F) a_s^{\overline{\text{MS}}}(\mu^2) \right] + \mathcal{O}(a_s^{\overline{\text{MS}^3}).\end{aligned}\quad (5.17)$$

Here the coefficients  $\delta a_{s,i}^{\overline{\text{MS}}}(N_F)$  are given by

$$\delta a_{s,1}^{\overline{\text{MS}}}(N_F) = \frac{2}{\varepsilon} \beta_0(N_F), \quad (5.18)$$

$$\delta a_{s,2}^{\overline{\text{MS}}}(N_F) = \frac{4}{\varepsilon^2} \beta_0^2(N_F) + \frac{1}{\varepsilon} \beta_1(N_F), \quad (5.19)$$

with  $\beta_k(N_F)$  the expansion coefficients of the QCD  $\beta$ -function [61, 62, 332–334]

$$\beta_0(N_F) = \frac{11}{3} C_A - \frac{4}{3} T_F N_F, \quad (5.20)$$

$$\beta_1(N_F) = \frac{34}{3} C_A^2 - 4 \left( \frac{5}{3} C_A + C_F \right) T_F N_F. \quad (5.21)$$

The renormalized gluon self-energy  $\Pi$  can be split into the purely light and the heavy flavor contributions,  $\Pi_L$  and  $\Pi_H$ ,

$$\Pi(p^2, m_1^2, m_2^2) = \Pi_L(p^2) + \Pi_H(p^2, m_1^2, m_2^2). \quad (5.22)$$

The heavy quarks are required to decouple from the running coupling constant and the renormalized OMEs for  $\mu^2 < m_1^2, m_2^2$  which implies [179]

$$\Pi_H(0, m_1^2, m_2^2) = 0. \quad (5.23)$$

Applying the background field method has the advantage of producing gauge-invariant results also for off-shell Green's functions. Applying the respective Feynman rules, cf. Ref. [70] and Appendix B, one obtains for the heavy flavor contributions to the unrenormalized gluon polarization function [329, 335]

$$\begin{aligned}\hat{\Pi}_{H,ab,\text{BF}}^{\mu\nu}(p^2, m_1^2, m_2^2, \mu^2, \varepsilon, \hat{a}_s) &= i(-p^2 g^{\mu\nu} + p^\mu p^\nu) \delta_{ab} \hat{\Pi}_{H,\text{BF}}(p^2, m_1^2, m_2^2, \mu^2, \varepsilon, \hat{a}_s), \quad (5.24) \\ \hat{\Pi}_{H,\text{BF}}(0, m_1^2, m_2^2, \mu^2, \varepsilon, \hat{a}_s) &= \hat{a}_s \frac{2\beta_{0,Q}}{\varepsilon} \left[ \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} + \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} \right] \exp\left( \sum_{i=2}^{\infty} \frac{\zeta_i}{i} \left( \frac{\varepsilon}{2} \right)^i \right) \\ &\quad + \hat{a}_s^2 \left[ \left( \frac{m_1^2}{\mu^2} \right)^\varepsilon + \left( \frac{m_2^2}{\mu^2} \right)^\varepsilon \right] \left[ \frac{1}{\varepsilon} \left( -\frac{20}{3} T_F C_A - 4 T_F C_F \right) \right. \\ &\quad \left. - \frac{32}{9} T_F C_A + 15 T_F C_F \right. \\ &\quad \left. + \varepsilon \left( -\frac{86}{27} T_F C_A - \frac{31}{4} T_F C_F - \frac{5}{3} \zeta_2 T_F C_A - \zeta_2 T_F C_F \right) \right]\end{aligned}$$

$$\begin{aligned}
 & +2 \left( \frac{2\beta_{0,Q}}{\varepsilon} \right)^2 \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} \exp \left( 2 \sum_{i=2}^{\infty} \frac{\zeta_i}{i} \left( \frac{\varepsilon}{2} \right)^i \right) \\
 & + \mathcal{O}(\hat{a}_s^3) ,
 \end{aligned} \tag{5.25}$$

where the masses  $m_1$  and  $m_2$  have been renormalized in the on-shell scheme, cf. Eq. (5.6). In order to write the relation in Eq. (5.25) in a more compact form the following notation

$$f(\varepsilon) \equiv \left[ \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} + \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} \right] \exp \left[ \sum_{i=2}^{\infty} \frac{\zeta_i}{i} \left( \frac{\varepsilon}{2} \right)^i \right] , \tag{5.26}$$

is used. The expression  $f(\varepsilon)$  is kept unexpanded in the dimensional regularization parameter  $\varepsilon$  for the moment. Furthermore, the contributions to the QCD  $\beta$ -function coefficients are denoted by  $\beta_{i,Q}^{(j)}$  [61, 62, 179, 182, 332–334]

$$\beta_{0,Q} = -\frac{4}{3} T_F , \tag{5.27}$$

$$\beta_{1,Q} = -4 \left( \frac{5}{3} C_A + C_F \right) T_F , \tag{5.28}$$

$$\beta_{1,Q}^{(1)} = -\frac{32}{9} T_F C_A + 15 T_F C_F , \tag{5.29}$$

$$\beta_{1,Q}^{(2)} = -\frac{86}{27} T_F C_A - \frac{31}{4} T_F C_F - \zeta_2 \left( \frac{5}{3} T_F C_A + T_F C_F \right) . \tag{5.30}$$

Eq. (5.25) differs from the sum of the two individual single-mass contributions [182] by the last term only, which is due to additional reducible Feynman diagrams in the cases of two heavy quark flavors of different mass.

The background field is renormalized using the  $Z$ -factor  $Z_A$  which is split into light and heavy quark contributions,  $Z_{A,L}$  and  $Z_{A,H}$ . It is related to the  $Z$ -factor renormalizing the coupling constant  $g$  via

$$Z_g = Z_A^{-\frac{1}{2}} = \frac{1}{(Z_{A,L} + Z_{A,H})^{1/2}} . \tag{5.31}$$

Concerning the light flavors, we require the renormalization to correspond to the  $\overline{\text{MS}}$ -scheme with  $N_F$  light flavors

$$Z_{A,l}(N_F) = Z_g^{\overline{\text{MS}}^{1/2}} . \tag{5.32}$$

The heavy flavor contributions are fixed by condition (5.23) which implies

$$\Pi_{H,\text{BF}}(0, \mu^2, a_s, m_1^2, m_2^2) + Z_{A,H} \equiv 0 . \tag{5.33}$$

The  $Z$ -factor in the MOM-scheme is read off by combining Eqs. (5.31),(5.23),(5.25) and (5.33)

$$Z_g^{\text{MOM}}(\varepsilon, N_F + 2, \mu, m_1^2, m_2^2) \equiv \frac{1}{(Z_{A,l} + Z_{A,H})^{1/2}} . \tag{5.34}$$

Up to  $\mathcal{O}(a_s^{\text{MOM}^3})$  one obtains the renormalization constant

$$\begin{aligned}
 Z_g^{\text{MOM}^2}(\varepsilon, N_F + 2, \mu, m_1^2, m_2^2) & = 1 + a_s^{\text{MOM}}(\mu^2) \left[ \frac{2}{\varepsilon} (\beta_0(N_F) + \beta_{0,Q} f(\varepsilon)) \right] \\
 & + a_s^{\text{MOM}^2}(\mu^2) \left[ \frac{\beta_1(N_F)}{\varepsilon} + \frac{4}{\varepsilon^2} (\beta_0(N_F) + \beta_{0,Q} f(\varepsilon))^2 \right]
 \end{aligned}$$

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$$\begin{aligned}
& + \frac{1}{\varepsilon} \left( \left( \frac{m_1^2}{\mu^2} \right)^\varepsilon + \left( \frac{m_2^2}{\mu^2} \right)^\varepsilon \right) \left( \beta_{1,Q} + \varepsilon \beta_{1,Q}^{(1)} + \varepsilon^2 \beta_{1,Q}^{(2)} \right) \\
& + \mathcal{O}(a_s^{\text{MOM}^3}) .
\end{aligned} \tag{5.35}$$

The coefficients of the MOM-scheme  $Z$ -factor,  $\delta a_{s,1}^{\text{MOM}}$  and  $\delta a_{s,2}^{\text{MOM}}$ , are defined analogously to those of the  $\overline{\text{MS}}$ -coefficients in Eq. (5.17)

$$\delta a_{s,1}^{\text{MOM}} = \frac{2\beta_0(N_F)}{\varepsilon} + \frac{2\beta_{0,Q}}{\varepsilon} f(\varepsilon) , \tag{5.36}$$

$$\begin{aligned}
\delta a_{s,2}^{\text{MOM}} &= \frac{\beta_1(N_F)}{\varepsilon} + \left( \frac{2\beta_0(N_F)}{\varepsilon} + \frac{2\beta_{0,Q}}{\varepsilon} f(\varepsilon) \right)^2 \\
&+ \frac{1}{\varepsilon} \left( \left( \frac{m_1^2}{\mu^2} \right)^\varepsilon + \left( \frac{m_2^2}{\mu^2} \right)^\varepsilon \right) \left( \beta_{1,Q} + \varepsilon \beta_{1,Q}^{(1)} + \varepsilon^2 \beta_{1,Q}^{(2)} \right) + \mathcal{O}(\varepsilon^2) .
\end{aligned} \tag{5.37}$$

Finally, we express our results in the  $\overline{\text{MS}}$ -scheme. For this transition the decoupling of the heavy quark flavors is assumed.

The transformation to the  $\overline{\text{MS}}$  scheme is then implied by

$$Z_g^{\overline{\text{MS}}^2}(\varepsilon, N_F + 2) a_s^{\overline{\text{MS}}}(\mu^2) = Z_g^{\text{MOM}^2}(\varepsilon, N_F + 2, \mu, m_1^2, m_2^2) a_s^{\text{MOM}}(\mu^2) . \tag{5.38}$$

Solving Eq. (5.38) perturbatively one obtains

$$\begin{aligned}
a_s^{\text{MOM}} &= a_s^{\overline{\text{MS}}} - \beta_{0,Q} \left( \ln \left( \frac{m_1^2}{\mu^2} \right) + \ln \left( \frac{m_2^2}{\mu^2} \right) \right) a_s^{\overline{\text{MS}}^2} + \left[ \beta_{0,Q}^2 \left( \ln \left( \frac{m_1^2}{\mu^2} \right) + \ln \left( \frac{m_2^2}{\mu^2} \right) \right)^2 \right. \\
&\quad \left. - \beta_{1,Q} \left( \ln \left( \frac{m_1^2}{\mu^2} \right) + \ln \left( \frac{m_2^2}{\mu^2} \right) \right) - 2\beta_{1,Q}^{(1)} \right] a_s^{\overline{\text{MS}}^3} + \mathcal{O} \left( a_s^{\overline{\text{MS}}^4} \right) ,
\end{aligned} \tag{5.39}$$

or,

$$\begin{aligned}
a_s^{\overline{\text{MS}}} &= a_s^{\text{MOM}} + a_s^{\text{MOM}^2} \left( \delta a_{s,1}^{\text{MOM}} - \delta a_{s,1}^{\overline{\text{MS}}}(N_F + 2) \right) + a_s^{\text{MOM}^3} \left( \delta a_{s,2}^{\text{MOM}} - \delta a_{s,2}^{\overline{\text{MS}}}(N_F + 2) \right. \\
&\quad \left. - 2\delta a_{s,1}^{\overline{\text{MS}}}(N_F + 2) \left[ \delta a_{s,1}^{\text{MOM}} - \delta a_{s,1}^{\overline{\text{MS}}}(N_F + 2) \right] \right) + \mathcal{O}(a_s^{\text{MOM}^4}) .
\end{aligned} \tag{5.40}$$

Note that, unlike in Eq. (5.17), in Eqs. (5.39) and (5.40)  $a_s^{\overline{\text{MS}}} \equiv a_s^{\overline{\text{MS}}}(N_F + 2)$ . Applying the coupling renormalization, cf. Eq. (5.35), to Eq. (5.15) the OME after mass and coupling renormalization is obtained

$$\begin{aligned}
\hat{A}_{ij} &= \delta_{ij} + a_s^{\text{MOM}} \hat{A}_{ij}^{(1)} + a_s^{\text{MOM}^2} \left[ \hat{A}_{ij}^{(2)} + \delta a_{s,1}^{\text{MOM}} \hat{A}_{ij}^{(1)} \right. \\
&\quad \left. + \delta m_1 \left( \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} m_1 \frac{d}{dm_1} + \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} m_2 \frac{d}{dm_2} \right) \hat{A}_{ij}^{(1)} \right] \\
&\quad + a_s^{\text{MOM}^3} \left[ \hat{A}_{ij}^{(3)} + \delta a_{s,2}^{\text{MOM}} \hat{A}_{ij}^{(1)} + 2\delta a_{s,1}^{\text{MOM}} \left[ \hat{A}_{ij}^{(2)} \right. \right. \\
&\quad \left. \left. + \delta m_1 \left( \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} m_1 \frac{d}{dm_1} + \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} m_2 \frac{d}{dm_2} \right) \hat{A}_{ij}^{(1)} \right] \right]
\end{aligned}$$

$$\begin{aligned}
 & +\delta m_1 \left[ \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} m_1 \frac{d}{dm_1} + \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} m_2 \frac{d}{dm_2} \right] \hat{A}_{ij}^{(2)} \\
 & + \left( \delta m_{2,1}(m_1, m_2) \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon} m_1 \frac{d}{dm_1} + \delta m_{2,2}(m_1, m_2) \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon} m_2 \frac{d}{dm_2} \right) \hat{A}_{ij}^{(1)} \\
 & + \frac{(\delta m_1)^2}{2} \left[ \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon} m_1^2 \frac{d^2}{dm_1^2} + \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon} m_2^2 \frac{d^2}{dm_2^2} \right] \hat{A}_{ij}^{(1)} \\
 & + (\delta m_1)^2 \left( \frac{m_1^2}{\mu^2} \right)^{\varepsilon/2} \left( \frac{m_2^2}{\mu^2} \right)^{\varepsilon/2} m_1 \frac{d}{dm_1} m_2 \frac{d}{dm_2} \hat{A}_{ij}^{(1)} \Big] , \tag{5.41}
 \end{aligned}$$

where the dependence on the masses,  $\varepsilon$  and  $N$  in the arguments of the OMEs has been suppressed for brevity.

### 5.3. Operator Renormalization

Next we remove the ultraviolet divergence of the different local operators defined in Eqs. (2.38-2.40) by introducing the respective  $Z$ -factors

$$O_{q,r;\mu_1,\dots,\mu_N}^{\text{NS}} = Z^{\text{NS}}(\mu^2) \hat{O}_{q,r;\mu_1,\dots,\mu_N}^{\text{NS}} , \tag{5.42}$$

$$O_{i;\mu_1,\dots,\mu_N}^{\text{S}} = Z_{ij}^{\text{S}}(\mu^2) \hat{O}_{j;\mu_1,\dots,\mu_N}^{\text{S}} , \quad i = q, g . \tag{5.43}$$

In the singlet case, the operator renormalization introduces a mixing between the different operators as they carry the same quantum numbers. Analogously to the OMEs, here the  $Z$ -factors are split into the flavor pure-singlet (PS) and non-singlet (NS) contributions

$$Z_{qq}^{-1} = Z_{qq}^{-1,\text{PS}} + Z_{qq}^{-1,\text{NS}} . \tag{5.44}$$

Each  $Z$ -factor is associated with an anomalous dimension  $\gamma_{ij}$  via

$$\gamma_{qq}^{\text{NS}}(a_s^{\overline{\text{MS}}}, N_F, N) = \mu \frac{d}{d\mu} \ln Z_{qq}^{\text{NS}}(a_s^{\overline{\text{MS}}}, N_F, \varepsilon, N) , \tag{5.45}$$

$$\gamma_{ij}(a_s^{\overline{\text{MS}}}, N_F, N) = \mu \frac{d}{d\mu} Z_{ij}(a_s^{\overline{\text{MS}}}, N_F, \varepsilon, N) . \tag{5.46}$$

Here both the anomalous dimensions and the operator  $Z$ -factors obey perturbative series expansions in the coupling constant

$$\gamma_{ij}^{\text{S, PS, NS}}(a_s^{\overline{\text{MS}}}, N_F, N) = \sum_{l=1}^{\infty} a_s^{\overline{\text{MS}} l} \gamma_{ij}^{(l-1),\text{S, PS, NS}}(N_F, N) \tag{5.47}$$

$$Z_{ij} = \delta_{ij} + \sum_{k=1}^{\infty} a_s^k Z_{ij}^{(k)} \tag{5.48}$$

$$Z_{ij}^{-1} = \delta_{ij} + \sum_{k=1}^{\infty} a_s^k Z_{ij}^{-1,(k)} . \tag{5.49}$$

In order to renormalize the respective operators, we first consider operator matrix elements with off-shell external legs as a sum of massive and massless contributions:

$$\begin{aligned}
 \hat{A}_{ij} \left( p^2, m_1^2, m_2^2, \mu^2, a_s^{\text{MOM}}, N_F + 2 \right) & = \hat{A}_{ij} \left( \frac{-p^2}{\mu^2}, a_s^{\overline{\text{MS}}}, N_F \right) \\
 & + \hat{A}_{ij}^{\text{Q}} \left( p^2, m_1^2, m_2^2, \mu^2, a_s^{\text{MOM}}, N_F + 2 \right) . \tag{5.50}
 \end{aligned}$$

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Here the massless contribution depends on  $a_s^{\overline{\text{MS}}}$  since the MOM-scheme, cf. Section 5.2, has been constructed in such a way that it corresponds to the  $\overline{\text{MS}}$ -scheme concerning the renormalization of the light quark flavor and gluon contributions.  $\hat{A}_{ij}^Q$  denotes any massive OME we consider. The term  $\delta_{ij}$ , which appears in the expansion of the OMEs (see Eqs. (5.15) and (5.41)), does not have any mass-dependence and is considered a part of the light flavor part  $\hat{A}_{ij}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\text{MS}}}, N_F\right)$ .

We first consider the renormalization of the purely massless contribution in the  $\overline{\text{MS}}$ -scheme [336]

$$A_{qq}^{\text{NS}}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\text{MS}}}, N_F, N\right) = Z_{qq}^{-1, \text{NS}}(a_s^{\overline{\text{MS}}}, N_F, \varepsilon, N) \hat{A}_{qq}^{\text{NS}}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\text{MS}}}, N_F, \varepsilon, N\right) \quad (5.51)$$

$$A_{ij}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\text{MS}}}, N_F, N\right) = Z_{il}^{-1}(a_s^{\overline{\text{MS}}}, N_F, \varepsilon, N) \hat{A}_{lj}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\text{MS}}}, N_F, \varepsilon, N\right), \quad i, j, l = q, g. \quad (5.52)$$

Solving Eqs. (5.45-5.46) yields the  $Z$ -factors in the singlet case

$$\begin{aligned} Z_{ij}(a_s^{\overline{\text{MS}}}, N_F) &= \delta_{ij} + a_s^{\overline{\text{MS}}} \frac{\gamma_{ij}^{(0)}}{\varepsilon} + a_s^{\overline{\text{MS}^2} \left\{ \frac{1}{\varepsilon^2} \left( \frac{1}{2} \gamma_{il}^{(0)} \gamma_{lj}^{(0)} + \beta_0 \gamma_{ij}^{(0)} \right) + \frac{1}{2\varepsilon} \gamma_{ij}^{(1)} \right\}} \\ &+ a_s^{\overline{\text{MS}^3} \left\{ \frac{1}{\varepsilon^3} \left( \frac{1}{6} \gamma_{il}^{(0)} \gamma_{lk}^{(0)} \gamma_{kj}^{(0)} + \beta_0 \gamma_{il}^{(0)} \gamma_{lj}^{(0)} + \frac{4}{3} \beta_0^2 \gamma_{ij}^{(0)} \right) \right. \\ &\left. + \frac{1}{\varepsilon^2} \left( \frac{1}{6} \gamma_{il}^{(1)} \gamma_{lj}^{(0)} + \frac{1}{3} \gamma_{il}^{(0)} \gamma_{lj}^{(1)} + \frac{2}{3} \beta_0 \gamma_{ij}^{(1)} + \frac{2}{3} \beta_1 \gamma_{ij}^{(0)} \right) + \frac{\gamma_{ij}^{(2)}}{3\varepsilon} \right\}. \end{aligned} \quad (5.53)$$

In the non-singlet and pure-singlet cases one has

$$\begin{aligned} Z_{qq}^{\text{NS}}(a_s^{\overline{\text{MS}}}, N_F) &= 1 + a_s^{\overline{\text{MS}}} \frac{\gamma_{qq}^{(0), \text{NS}}}{\varepsilon} + a_s^{\overline{\text{MS}^2} \left\{ \frac{1}{\varepsilon^2} \left( \frac{1}{2} \gamma_{qq}^{(0), \text{NS}^2} + \beta_0 \gamma_{qq}^{(0), \text{NS}} \right) + \frac{1}{2\varepsilon} \gamma_{qq}^{(1), \text{NS}} \right\}} \\ &+ a_s^{\overline{\text{MS}^3} \left\{ \frac{1}{\varepsilon^3} \left( \frac{1}{6} \gamma_{qq}^{(0), \text{NS}^3} + \beta_0 \gamma_{qq}^{(0), \text{NS}^2} + \frac{4}{3} \beta_0^2 \gamma_{qq}^{(0), \text{NS}} \right) \right. \\ &\left. + \frac{1}{\varepsilon^2} \left( \frac{1}{2} \gamma_{qq}^{(0), \text{NS}} \gamma_{qq}^{(1), \text{NS}} + \frac{2}{3} \beta_0 \gamma_{qq}^{(1), \text{NS}} + \frac{2}{3} \beta_1 \gamma_{qq}^{(0), \text{NS}} \right) + \frac{1}{3\varepsilon} \gamma_{qq}^{(2), \text{NS}} \right\} \end{aligned} \quad (5.54)$$

$$\begin{aligned} Z_{qq}^{\text{PS}}(a_s^{\overline{\text{MS}}}, N_F) &= a_s^{\overline{\text{MS}^2} \left\{ \frac{1}{2\varepsilon^2} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} + \frac{1}{2\varepsilon} \gamma_{qq}^{(1), \text{PS}} \right\}} + a_s^{\overline{\text{MS}^3} \left\{ \frac{1}{\varepsilon^3} \left( \frac{1}{3} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \right) \right. \\ &+ \frac{1}{6} \gamma_{qq}^{(0)} \gamma_{gg}^{(0)} \gamma_{qq}^{(0)} + \beta_0 \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \left. \right\}} + \frac{1}{\varepsilon^2} \left( \frac{1}{3} \gamma_{qq}^{(0)} \gamma_{qq}^{(1)} \right) \\ &+ \frac{1}{6} \gamma_{qq}^{(1)} \gamma_{qq}^{(0)} + \frac{1}{2} \gamma_{qq}^{(0)} \gamma_{qq}^{(1), \text{PS}} + \frac{2}{3} \beta_0 \gamma_{qq}^{(1), \text{PS}} \left. \right\} + \frac{\gamma_{qq}^{(2), \text{PS}}}{3\varepsilon}, \end{aligned} \quad (5.55)$$

respectively. The  $Z$ -factors describing the ultraviolet renormalization of the complete operator matrix elements  $\hat{A}_{ij}(p^2, m_1^2, m_2^2, \mu^2, a_s^{\text{MOM}}, N_F + 2)$  are obtained by inverting Eqs. (5.53-5.55) and replacing  $N_F \rightarrow N_F + 2$ . Finally, the transformation in Eq. (5.40) is applied. The resulting operator  $Z$ -factors read:

$$\begin{aligned} Z_{ij}^{-1}(a_s^{\text{MOM}}, N_F + 2, \mu) &= \delta_{ij} - a_s^{\text{MOM}} \frac{\gamma_{ij}^{(0)}}{\varepsilon} + a_s^{\text{MOM}^2} \left[ \frac{1}{\varepsilon} \left( -\frac{1}{2} \gamma_{ij}^{(1)} - \delta a_{s,1}^{\text{MOM}} \gamma_{ij}^{(0)} \right) \right. \\ &\left. + \frac{1}{\varepsilon^2} \left( \frac{1}{2} \gamma_{il}^{(0)} \gamma_{lj}^{(0)} + \beta_0 \gamma_{ij}^{(0)} \right) \right] + a_s^{\text{MOM}^3} \left[ \frac{1}{\varepsilon} \left( -\frac{1}{3} \gamma_{ij}^{(2)} - \delta a_{s,1}^{\text{MOM}} \gamma_{ij}^{(1)} \right) \right. \end{aligned}$$



$$\begin{aligned}
 & -\delta a_{s,2}^{\text{MOM}} \gamma_{ij}^{(0)}) + \frac{1}{\varepsilon^2} \left( \frac{4}{3} \beta_0 \gamma_{ij}^{(1)} + 2\delta a_{s,1}^{\text{MOM}} \beta_0 \gamma_{ij}^{(0)} + \frac{1}{3} \beta_1 \gamma_{ij}^{(0)} \right. \\
 & + \delta a_{s,1}^{\text{MOM}} \gamma_{il}^{(0)} \gamma_{lj}^{(0)} + \frac{1}{3} \gamma_{il}^{(1)} \gamma_{lj}^{(0)} + \frac{1}{6} \gamma_{il}^{(0)} \gamma_{lj}^{(1)} \left. \right) + \frac{1}{\varepsilon^3} \left( -\frac{4}{3} \beta_0^2 \gamma_{ij}^{(0)} \right. \\
 & \left. - \beta_0 \gamma_{il}^{(0)} \gamma_{lj}^{(0)} - \frac{1}{6} \gamma_{il}^{(0)} \gamma_{lk}^{(0)} \gamma_{kj}^{(0)} \right) \Big], \tag{5.56}
 \end{aligned}$$

$$\begin{aligned}
 Z_{qq}^{-1,\text{NS}}(a_s^{\text{MOM}}, N_F + 2) &= 1 - a_s^{\text{MOM}} \frac{\gamma_{qq}^{(0),\text{NS}}}{\varepsilon} + a_s^{\text{MOM}^2} \left[ \frac{1}{\varepsilon} \left( -\frac{1}{2} \gamma_{qq}^{(1),\text{NS}} - \delta a_{s,1}^{\text{MOM}} \gamma_{qq}^{(0),\text{NS}} \right) \right. \\
 & + \frac{1}{\varepsilon^2} \left( \beta_0 \gamma_{qq}^{(0),\text{NS}} + \frac{1}{2} \gamma_{qq}^{(0),\text{NS}^2} \right) \Big] + a_s^{\text{MOM}^3} \left[ \frac{1}{\varepsilon} \left( -\frac{1}{3} \gamma_{qq}^{(2),\text{NS}} - \delta a_{s,1}^{\text{MOM}} \gamma_{qq}^{(1),\text{NS}} \right. \right. \\
 & - \delta a_{s,2}^{\text{MOM}} \gamma_{qq}^{(0),\text{NS}} \left. \right) + \frac{1}{\varepsilon^2} \left( \frac{4}{3} \beta_0 \gamma_{qq}^{(1),\text{NS}} + 2\delta a_{s,1}^{\text{MOM}} \beta_0 \gamma_{qq}^{(0),\text{NS}} + \frac{1}{3} \beta_1 \gamma_{qq}^{(0),\text{NS}} \right. \\
 & + \frac{1}{2} \gamma_{qq}^{(0),\text{NS}} \gamma_{qq}^{(1),\text{NS}} + \delta a_{s,1}^{\text{MOM}} \gamma_{qq}^{(0),\text{NS}^2} \left. \right) + \frac{1}{\varepsilon^3} \left( -\frac{4}{3} \beta_0^2 \gamma_{qq}^{(0),\text{NS}} - \beta_0 \gamma_{qq}^{(0),\text{NS}^2} \right. \\
 & \left. \left. - \frac{1}{6} \gamma_{qq}^{(0),\text{NS}^3} \right) \right], \tag{5.57}
 \end{aligned}$$

$$\begin{aligned}
 Z_{qq}^{-1,\text{PS}}(a_s^{\text{MOM}}, N_F + 2) &= a_s^{\text{MOM}^2} \left[ \frac{1}{\varepsilon} \left( -\frac{1}{2} \gamma_{qq}^{(1),\text{PS}} \right) + \frac{1}{\varepsilon^2} \left( \frac{1}{2} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \right) \right] + a_s^{\text{MOM}^3} \left[ \frac{1}{\varepsilon} \left( -\frac{1}{3} \gamma_{qq}^{(2),\text{PS}} \right. \right. \\
 & - \delta a_{s,1}^{\text{MOM}} \gamma_{qq}^{(1),\text{PS}} \left. \right) + \frac{1}{\varepsilon^2} \left( \frac{1}{6} \gamma_{qq}^{(0)} \gamma_{qq}^{(1)} + \frac{1}{3} \gamma_{qq}^{(0)} \gamma_{qq}^{(1)} + \frac{1}{2} \gamma_{qq}^{(0)} \gamma_{qq}^{(1)} \right. \\
 & + \frac{4}{3} \beta_0 \gamma_{qq}^{(1),\text{PS}} + \delta a_{s,1}^{\text{MOM}} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \left. \right) + \frac{1}{\varepsilon^3} \left( -\frac{1}{3} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} - \frac{1}{6} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \right. \\
 & \left. \left. - \beta_0 \gamma_{qq}^{(0)} \gamma_{qq}^{(0)} \right) \right]. \tag{5.58}
 \end{aligned}$$

Here and in the Eqs. (5.53-5.55) the  $N_F$ -dependence of the anomalous dimensions  $\gamma_{ij}$  and  $\beta_i$  has been dropped for brevity. The inverse  $Z$ -factors for the purely light-parton case correspond to Eqs. (5.56-5.58) after substituting  $N_F + 2 \rightarrow N_F$  and  $\delta a_{s,i}^{\text{MOM}} \rightarrow \delta a_{s,i}^{\overline{\text{MS}}}$ .

Since only the ultraviolet renormalization for the massive contributions to the operator matrix element in Eq. (5.50) shall be performed the contributions stemming from purely light parts are subtracted again

$$\begin{aligned}
 \tilde{A}_{ij}^Q(p^2, m_1^2, m_2^2, \mu^2, a_s^{\text{MOM}}, N_F + 2) &= Z_{il}^{-1}(a_s^{\text{MOM}}, N_F + 2, \mu) \hat{A}_{ij}^Q(p^2, m_1^2, m_2^2, \mu^2, a_s^{\text{MOM}}, N_F + 2) \\
 & + Z_{il}^{-1}(a_s^{\text{MOM}}, N_F + 2, \mu) \hat{A}_{ij} \left( \frac{-p^2}{\mu^2}, a_s^{\overline{\text{MS}}}, N_F \right) \\
 & - Z_{il}^{-1}(a_s^{\overline{\text{MS}}}, N_F, \mu) \hat{A}_{ij} \left( \frac{-p^2}{\mu^2}, a_s^{\overline{\text{MS}}}, N_F \right). \tag{5.59}
 \end{aligned}$$

Finally, the limit  $p^2 \rightarrow 0$  is performed. Since scale-less diagrams vanish if computed in dimensional regularization, only the Born piece of the massless OME contributes

$$\hat{A}_{ij} \left( 0, \alpha_s^{\overline{\text{MS}}}, N_F \right) = \delta_{ij}. \tag{5.60}$$

One obtains the UV-renormalization prescription

$$\tilde{A}_{ij}^Q \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, a_s^{\text{MOM}}, N_F + 2 \right) = a_s^{\text{MOM}} \left( \hat{A}_{ij}^{(1),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + Z_{ij}^{-1,(1)}(N_F + 2, \mu) - Z_{ij}^{-1,(1)}(N_F) \right)$$

$$\begin{aligned}
 & + a_s^{\text{MOM}^2} \left( \hat{A}_{ij}^{(2),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + Z_{ij}^{-1,(2)}(N_F + 2, \mu) - Z_{ij}^{-1,(2)}(N_F) \right. \\
 & \left. + Z_{ik}^{-1,(1)}(N_F + 2, \mu) \hat{A}_{kj}^{(1),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right) \\
 & + a_s^{\text{MOM}^3} \left( \hat{A}_{ij}^{(3),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + Z_{ij}^{-1,(3)}(N_F + 2, \mu) \right. \\
 & \left. - Z_{ij}^{-1,(3)}(N_F) + Z_{ik}^{-1,(1)}(N_F + 2, \mu) \hat{A}_{kj}^{(2),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right. \\
 & \left. + Z_{ik}^{-1,(2)}(N_F + 2, \mu) \hat{A}_{kj}^{(1),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right). \quad (5.61)
 \end{aligned}$$

Here  $Z$ -factors at  $N_F + 2$  flavors describe the massive case, cf. Eqs. (5.56-5.58), while those with argument  $N_F$  denote the  $Z$ -factors for the massless case.

## 5.4. Collinear Factorization

At this point only collinear singularities remain. They arise from massless subgraphs only and are therefore independent of the additional heavy quark flavor considered in these analyses. Thus [182] can be followed directly to remove the collinear singularities via mass factorization

$$A_{ij} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, a_s^{\text{MOM}}, N_F + 2 \right) = \tilde{A}_{il}^Q \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, a_s^{\text{MOM}}, N_F + 2 \right) \Gamma_{lj}^{-1}. \quad (5.62)$$

In a fully massless scenario the transition functions  $\Gamma_{ij}$  would be related to the light flavor renormalization constant via

$$\Gamma_{ij}(N_F) = Z_{ij}^{-1}(N_F), \quad (5.63)$$

cf. Ref. [179]. However, in the presence of one or more heavy quark flavors the transition functions stem from the corresponding massless subgraphs only. Due to this and the subtraction of the  $\delta_{ij}$ -term in the OMEs after ultraviolet renormalization  $\tilde{A}_{ij}^Q$  the transition functions contribute up to  $\mathcal{O}(\alpha_s^2)$  only.

The renormalized OME is then obtained by

$$\begin{aligned}
 & A_{ij} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}, a_s^{\text{MOM}}, N_F + 2 \right) = \\
 & a_s^{\text{MOM}} \left( \hat{A}_{ij}^{(1),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + Z_{ij}^{-1,(1)}(N_F + 2) - Z_{ij}^{-1,(1)}(N_F) \right) \\
 & + a_s^{\text{MOM}^2} \left( \hat{A}_{ij}^{(2),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + Z_{ij}^{-1,(2)}(N_F + 2) - Z_{ij}^{-1,(2)}(N_F) \right. \\
 & \quad \left. + Z_{ik}^{-1,(1)}(N_F + 2) \hat{A}_{kj}^{(1),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + \left[ \hat{A}_{il}^{(1),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + Z_{il}^{-1,(1)}(N_F + 2) \right. \right. \\
 & \quad \left. \left. - Z_{il}^{-1,(1)}(N_F) \right] \Gamma_{lj}^{-1,(1)}(N_F) \right) \\
 & + a_s^{\text{MOM}^3} \left( \hat{A}_{ij}^{(3),Q} \left( \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + Z_{ij}^{-1,(3)}(N_F + 2) - Z_{ij}^{-1,(3)}(N_F) \right)
 \end{aligned}$$

$$\begin{aligned}
 & + Z_{ik}^{-1,(1)}(N_F + 2)\hat{A}_{kj}^{(2),Q}\left(\frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) + Z_{ik}^{-1,(2)}(N_F + 2)\hat{A}_{kj}^{(1),Q}\left(\frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) \\
 & + \left[\hat{A}_{il}^{(1),Q}\left(\frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) + Z_{il}^{-1,(1)}(N_F + 2) - Z_{il}^{-1,(1)}(N_F)\right]\Gamma_{lj}^{-1,(2)}(N_F) \\
 & + \left[\hat{A}_{il}^{(2),Q}\left(\frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right) + Z_{il}^{-1,(2)}(N_F + 2) - Z_{il}^{-1,(2)}(N_F)\right. \\
 & \left. + Z_{ik}^{-1,(1)}(N_F + 2)\hat{A}_{kl}^{(1),Q}\left(\frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2}\right)\right]\Gamma_{lj}^{-1,(1)}(N_F) \Big) + O\left(a_s^{\text{MOM}^4}\right). \quad (5.64)
 \end{aligned}$$

Eq. (5.64) differs from the corresponding renormalization and factorization prescription for one heavy quark flavor [182] only by the definition of the renormalization constants  $Z_{ij}^{-1,(k)}(N_F + 2)$ . Now the term  $\delta_{ij}$  is added back to the massive OME. In a final step, the coupling constant is transformed to that in the  $\overline{\text{MS}}$ -scheme via Eq. (5.39).

## 5.5. One-particle reducible contributions

The renormalization of the massive operator matrix elements is based on the complete set of Feynman diagrams which also includes the one-particle reducible contributions. These terms contribute from  $\mathcal{O}(a_s^2)$  onward and are obtained by quark and gluon self-energy contributions to the external legs of lower order one-particle irreducible diagrams. From 3-loop order onward the reducible contributions to the OMEs  $A_{Qg}$  and  $A_{gg,Q}$  may contain three different heavy flavors, while this is not the case for the irreducible contributions. Note that the inclusion of the top quark in a loop of the irreducible terms for  $A_{ij}^{(3)}$  would demand to consider the energy range  $Q^2 \gg m_t^2$ . At a scale  $\mu^2 \simeq m_t^2$ , both charm and bottom can be dealt with as effectively massless. The emergence of massive top loops in the reducible contributions is accounted for by renormalization. In the following we will strictly consider the case of two heavy flavors only.

### Self-energy contributions

The scalar self-energies are obtained by projecting out the Lorentz-structure

$$\hat{\Pi}_{\mu\nu}^{ab}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2, \hat{a}_s) = i\delta^{ab} [-g_{\mu\nu}p^2 + p_\mu p_\nu] \hat{\Pi}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2, \hat{a}_s), \quad (5.65)$$

$$\hat{\Pi}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2, \hat{a}_s) = \sum_{k=1}^{\infty} \hat{a}_s^k \hat{\Pi}^{(k)}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2), \quad (5.66)$$

$$\hat{\Sigma}_{ij}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2, \hat{a}_s) = i\delta_{ij} \not{p} \hat{\Sigma}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2, \hat{a}_s), \quad (5.67)$$

$$\hat{\Sigma}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2, \hat{a}_s) = \sum_{k=2}^{\infty} \hat{a}_s^k \hat{\Sigma}^{(k)}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2). \quad (5.68)$$

In the same way as the OMEs themselves the irreducible two-mass self-energies can be divided into contributions which depend on one mass only and an additional part stemming from diagrams containing both heavy quark flavors

$$\hat{\Pi}^{(k)}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2) = \hat{\Pi}^{(k)}\left(p^2, \frac{\hat{m}_1^2}{\mu^2}\right) + \hat{\Pi}^{(k)}\left(p^2, \frac{\hat{m}_2^2}{\mu^2}\right) + \hat{\hat{\Pi}}^{(k)}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2), \quad (5.69)$$

$$\hat{\Sigma}^{(j)}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2) = \hat{\Sigma}^{(j)}\left(p^2, \frac{\hat{m}_1^2}{\mu^2}\right) + \hat{\Sigma}^{(j)}\left(p^2, \frac{\hat{m}_2^2}{\mu^2}\right) + \hat{\hat{\Sigma}}^{(j)}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2). \quad (5.70)$$

Up to two-loop order no diagrams with two heavy flavors contribute

$$\hat{\Pi}^{(k)}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2) = 0 \text{ for } k \in \{1, 2\}, \quad (5.71)$$

$$\hat{\Sigma}^{(2)}(p^2, \hat{m}_1^2, \hat{m}_2^2, \mu^2) = 0. \quad (5.72)$$

The single-mass contributions for the gluon are known from [182, 337–339]

$$\hat{\Pi}^{(1)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) = T_F \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2} \left[ -\frac{8}{3\varepsilon} \exp\left(\sum_{i=2}^{\infty} \frac{\zeta_i}{i} \left(\frac{\varepsilon}{2}\right)^i\right) \right], \quad (5.73)$$

$$\begin{aligned} \hat{\Pi}^{(2)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) &= T_F \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon} \left\{ -\frac{4}{\varepsilon^2} C_A + \frac{1}{\varepsilon} (5C_A - 12C_F) + C_A \left(\frac{13}{12} - \zeta_2\right) - \frac{13}{3} C_F \right. \\ &\quad \left. + \varepsilon \left[ C_A \left(\frac{169}{144} + \frac{5}{4} \zeta_2 - \frac{\zeta_3}{3}\right) - C_F \left(\frac{35}{12} + 3\zeta_2\right) \right] \right\} + \mathcal{O}(\varepsilon^2), \end{aligned} \quad (5.74)$$

$$\begin{aligned} \hat{\Pi}^{(3)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) &= T_F \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2} \left\{ \frac{1}{\varepsilon^3} \left[ -\frac{32}{9} T_F C_A (2N_F + 1) + \frac{164}{9} C_A^2 \right] \right. \\ &\quad + \frac{1}{\varepsilon^2} \left[ \frac{80}{27} (C_A - 6C_F) N_F T_F + \frac{8}{27} (35C_A - 48C_F) T_F - \frac{781}{27} C_A^2 \right. \\ &\quad \left. + \frac{712}{9} C_A C_F \right] + \frac{1}{\varepsilon} \left[ \frac{4}{27} (C_A(-101 - 18\zeta_2) - 62C_F) N_F T_F \right. \\ &\quad \left. - \frac{2}{27} (C_A(37 + 18\zeta_2) + 80C_F) T_F + C_A^2 \left(-12\zeta_3 + \frac{41}{6} \zeta_2 + \frac{3181}{108}\right) \right. \\ &\quad \left. + C_A C_F \left(16\zeta_3 - \frac{1570}{27}\right) + \frac{272}{3} C_F^2 \right] \\ &\quad + N_F T_F \left[ C_A \left(\frac{56}{9} \zeta_3 + \frac{10}{9} \zeta_2 - \frac{3203}{243}\right) - C_F \left(\frac{20}{3} \zeta_2 + \frac{1942}{81}\right) \right] \\ &\quad + T_F \left[ C_A \left(-\frac{295}{18} \zeta_3 + \frac{35}{9} \zeta_2 + \frac{6361}{486}\right) - C_F \left(7\zeta_3 + \frac{16}{3} \zeta_2 + \frac{218}{81}\right) \right] \\ &\quad + C_A^2 \left(4B_4 - 27\zeta_4 + \frac{1969}{72} \zeta_3 - \frac{781}{72} \zeta_2 + \frac{42799}{3888}\right) \\ &\quad + C_A C_F \left(-8B_4 + 36\zeta_4 - \frac{1957}{12} \zeta_3 + \frac{89}{3} \zeta_2 + \frac{10633}{81}\right) \\ &\quad \left. + C_F^2 \left(\frac{95}{3} \zeta_3 + \frac{274}{9}\right) \right\} + \mathcal{O}(\varepsilon), \end{aligned} \quad (5.75)$$

and for the quark self-energy,

$$\hat{\Sigma}^{(2)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) = T_F C_F \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon} \left[ \frac{2}{\varepsilon} + \frac{5}{6} + \left(\frac{89}{72} + \frac{\zeta_2}{2}\right) \varepsilon \right] + \mathcal{O}(\varepsilon^2). \quad (5.76)$$

$$\begin{aligned} \hat{\Sigma}^{(3)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) &= T_F C_F \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2} \left\{ \frac{8}{3\varepsilon^3} C_A + \frac{1}{\varepsilon^2} \left[ \frac{32}{9} T_F (N_F + 2) - \frac{40}{9} C_A - \frac{8}{3} C_F \right] \right. \\ &\quad \left. + \frac{1}{\varepsilon} \left[ \frac{40}{27} T_F (N_F + 2) + C_A \left(\zeta_2 + \frac{454}{27}\right) - 26C_F \right] \right. \\ &\quad \left. + N_F T_F \left(\frac{4}{3} \zeta_2 + \frac{674}{81}\right) + T_F \left(\frac{8}{3} \zeta_2 + \frac{604}{81}\right) + C_A \left(\frac{17}{3} \zeta_3 - \frac{5}{3} \zeta_2 + \frac{1879}{162}\right) \right\} \end{aligned}$$

$$-C_F \left( 8\zeta_3 + \zeta_2 + \frac{335}{18} \right) \Big\} + \mathcal{O}(\varepsilon). \quad (5.77)$$

Similarly to other massive processes [182, 340–344] the constant

$$B_4 = -4\zeta_2 \ln^2(2) + \frac{2}{3} \ln^4(2) - \frac{13}{2} \zeta_4 + 16\text{Li}_4\left(\frac{1}{2}\right) \approx -1.762800093... \quad (5.78)$$

emerges in Eq. (5.75). At  $\mathcal{O}(\alpha_s^3)$  irreducible diagrams with two different masses contribute for the first time. In [202] the gluonic case was calculated to  $\mathcal{O}(\eta^3)$  using the codes `Q2E/Exp`[200, 201]. However, the full  $\eta$  dependence is needed in the following. All the diagrams can be expressed through a one-dimensional Mellin-Barnes integral and the residue sums are easily evaluated using the `Mathematica` package `EvaluateMultiSums` [271] which is build on `Sigma` [268, 269] and `HarmonicSums` [273, 274]. The result is given by [9, 345]

$$\begin{aligned} \hat{\Pi}^{(3)}(0, m_1^2, m_2^2, \mu^2) = & C_F T_F^2 \left\{ \frac{256}{9\varepsilon^2} + \frac{64}{3\varepsilon} \left[ L_1 + L_2 + \frac{5}{9} \right] - 5\eta - \frac{5}{\eta} \right. \\ & + \left( -\frac{5\eta}{8} - \frac{5}{8\eta} + \frac{51}{4} \right) \ln^2(\eta) + \left( \frac{5}{2\eta} - \frac{5\eta}{2} \right) \ln(\eta) + \frac{32\zeta_2}{3} \\ & + 32L_1L_2 + \frac{80}{9}L_1 + \frac{80}{9}L_2 + \frac{1246}{81} \\ & + \left( \frac{5\eta^{3/2}}{2} + \frac{5}{2\eta^{3/2}} + \frac{3\sqrt{\eta}}{2} + \frac{3}{2\sqrt{\eta}} \right) \left[ \frac{1}{8} \ln\left(\frac{1+\sqrt{\eta}}{1-\sqrt{\eta}}\right) \ln^2(\eta) \right. \\ & \left. \left. - \text{Li}_3(-\sqrt{\eta}) + \text{Li}_3(\sqrt{\eta}) - \frac{1}{2} \ln(\eta) (\text{Li}_2(\sqrt{\eta}) - \text{Li}_2(-\sqrt{\eta})) \right] \right\} \\ & - C_A T_F^2 \left\{ \frac{64}{9\varepsilon^3} + \frac{16}{3\varepsilon^2} \left[ (L_1 + L_2) - \frac{35}{9} \right] + \frac{4}{\varepsilon} \left[ L_1^2 + L_2^2 - \frac{35}{9} L_1 \right. \right. \\ & \left. \left. - \frac{35}{9} L_2 + \frac{2}{3} \zeta_2 + \frac{37}{27} \right] + 2(L_1^3 + L_2^3) - \frac{70}{3} L_1 L_2 - \frac{4}{9} \ln^3(\eta) \right. \\ & + \left( 2\zeta_2 + \frac{37}{9} \right) (L_1 + L_2) + \left[ \frac{8}{3} \ln(1-\eta) - \frac{2}{3} \left( \eta + \frac{1}{\eta} \right) - \frac{179}{18} \right] \\ & \times \ln^2(\eta) - \frac{16}{3} \left( \eta + \frac{1}{\eta} \right) - \frac{70}{9} \zeta_2 - \frac{56}{9} \zeta_3 - \frac{3769}{243} \\ & + \frac{8}{3} \left( \frac{1}{\eta} - \eta \right) \ln(\eta) + \frac{16}{3} (\text{Li}_2(\eta) \ln(\eta) - \text{Li}_3(\eta)) \\ & + \left[ 8 \frac{1+\eta^3}{3\eta^{3/2}} + 10 \frac{1+\eta}{\sqrt{\eta}} \right] \left[ \frac{1}{8} \ln\left(\frac{1+\sqrt{\eta}}{1-\sqrt{\eta}}\right) \ln^2(\eta) - \text{Li}_3(-\sqrt{\eta}) \right. \\ & \left. \left. + \text{Li}_3(\sqrt{\eta}) - \frac{1}{2} \ln(\eta) (\text{Li}_2(\sqrt{\eta}) - \text{Li}_2(-\sqrt{\eta})) \right] + \mathcal{O}(\varepsilon) \right\}. \quad (5.79) \end{aligned}$$

After the completion of the calculation given in Ref. [9] the paper [345] was brought to our attention. Here the same quantity can be inferred implicitly. After adjusting notations complete agreement is found. The quarkonic self-energy contributions have been computed analytically in  $\eta$ , one obtains

$$\begin{aligned} \hat{\Sigma}^{(3)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2) = & T_F^2 C_F \left( \frac{\hat{m}_1 \hat{m}_2}{\mu^2} \right)^{\frac{3}{2}\varepsilon} \left[ \frac{128}{9\varepsilon^2} + \frac{160}{27\varepsilon} + \frac{4}{3} \ln^2(\eta) + \frac{16}{3} \zeta_2 \right. \\ & \left. + \frac{1208}{81} + \mathcal{O}(\varepsilon) \right]. \quad (5.80) \end{aligned}$$

**The reducible operator matrix elements**

As in Eqs. (5.69-5.70) the two-mass OMEs at one-loop order and the irreducible OMEs at  $\mathcal{O}(\alpha_s^2)$  are defined by

$$\hat{A}_{ij}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) = \hat{A}_{ij}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}\right) + \hat{A}_{ij}^{(1)}\left(\frac{\hat{m}_2^2}{\mu^2}\right), \quad (5.81)$$

$$\hat{A}_{ij}^{(\prime),(2),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) = \hat{A}_{ij}^{(\prime),(2),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}\right) + \hat{A}_{ij}^{(\prime),(2),\text{irr}}\left(\frac{\hat{m}_2^2}{\mu^2}\right), \quad (5.82)$$

where the  $A_{ij}$ 's with one argument denote the usual single-mass OMEs. The irreducible contributions from OMEs with external gluons need a further discussion. These have to be included using a consistent projection, either physical, cf. Eq. (2.83), or unphysical, cf. Eq. (2.84), since the ghost contributions restore gauge invariance globally. Therefore a  $\prime$  is included for irreducible OMEs with external gluons. Using the definitions in Eqs. (5.69-5.70) and in Eqs. (5.81-5.82) the reducible massive operator matrix elements at  $\mathcal{O}(\alpha_s^2)$  are composed by

$$\hat{A}_{qq}^{(2),\text{NS}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) = \hat{A}_{qq}^{(2),\text{NS},\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) - \hat{\Sigma}^{(2)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2), \quad (5.83)$$

$$\hat{A}_{Qg}^{(2)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) = \hat{A}_{Qg}^{\prime,(2),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) - \hat{A}_{Qg}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) \hat{\Pi}^{(1)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2), \quad (5.84)$$

$$\begin{aligned} \hat{A}_{gg}^{(2)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) &= \hat{A}_{gg}^{\prime,(2),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) - \hat{\Pi}^{(2)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2) \\ &\quad - \hat{A}_{gg}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) \hat{\Pi}^{(1)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2), \end{aligned} \quad (5.85)$$

and at  $\mathcal{O}(\alpha_s^3)$  by

$$\hat{A}_{qq}^{(3),\text{NS}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) = \hat{A}_{qq}^{(3),\text{NS},\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) - \hat{\Sigma}^{(3)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2) \quad (5.86)$$

$$\begin{aligned} \hat{A}_{Qg}^{(3)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) &= \hat{A}_{Qg}^{\prime,(3),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) - \hat{A}_{Qg}^{(2)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) \hat{\Pi}^{(1)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2) \\ &\quad - \hat{A}_{Qg}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) \hat{\Pi}^{(2)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2) \end{aligned} \quad (5.87)$$

$$\begin{aligned} \hat{A}_{gg}^{(3)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) &= \hat{A}_{gg}^{\prime,(3),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) - \hat{A}_{gg}^{(2)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) \hat{\Pi}^{(1)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2) \\ &\quad - \hat{A}_{gg}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) \hat{\Pi}^{(2)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2) - \hat{\Pi}^{(3)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2). \end{aligned} \quad (5.88)$$

One can subtract the single-mass contributions to these equations using Eq. (5.1), keeping only the genuine two-mass contributions. At three loops one obtains

$$\hat{A}_{qq}^{(3),\text{NS}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) = \hat{A}_{qq}^{(3),\text{NS},\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) - \hat{\Sigma}^{(3)}(0, \hat{m}_1^2, \hat{m}_2^2, \mu^2) \quad (5.89)$$

$$\begin{aligned} \hat{A}_{Qg}^{(3)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) &= \hat{A}_{Qg}^{\prime,(3),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) \\ &\quad + \hat{A}_{Qg}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}\right) \left[ 2\hat{\Pi}^{(1)}\left(0, \frac{\hat{m}_1^2}{\mu^2}\right) + \hat{\Pi}^{(1)}\left(0, \frac{\hat{m}_2^2}{\mu^2}\right) \right] \hat{\Pi}^{(1)}\left(0, \frac{\hat{m}_2^2}{\mu^2}\right) \\ &\quad + \hat{A}_{Qg}^{(1)}\left(\frac{\hat{m}_2^2}{\mu^2}\right) \left[ 2\hat{\Pi}^{(1)}\left(0, \frac{\hat{m}_2^2}{\mu^2}\right) + \hat{\Pi}^{(1)}\left(0, \frac{\hat{m}_1^2}{\mu^2}\right) \right] \hat{\Pi}^{(1)}\left(0, \frac{\hat{m}_1^2}{\mu^2}\right) \end{aligned}$$

$$\begin{aligned}
 & -\hat{A}_{Qg}^{(2)}\left(\frac{\hat{m}_1^2}{\mu^2}\right)\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_2^2}{\mu^2}\right)-\hat{A}_{Qg}^{(2)}\left(\frac{\hat{m}_2^2}{\mu^2}\right)\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_1^2}{\mu^2}\right) \\
 & -\hat{A}_{Qg}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}\right)\hat{\Pi}^{(2)}\left(0,\frac{\hat{m}_2^2}{\mu^2}\right)-\hat{A}_{Qg}^{(1)}\left(\frac{\hat{m}_2^2}{\mu^2}\right)\hat{\Pi}^{(2)}\left(0,\frac{\hat{m}_1^2}{\mu^2}\right)
 \end{aligned} \tag{5.90}$$

$$\begin{aligned}
 \hat{A}_{gg}^{(3)}\left(\frac{\hat{m}_1^2}{\mu^2},\frac{\hat{m}_2^2}{\mu^2}\right) &= \hat{A}_{gg}^{(3),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2},\frac{\hat{m}_2^2}{\mu^2}\right)-\hat{\Pi}^{(3)}\left(0,\hat{m}_1^2,\hat{m}_2^2,\mu^2\right) \\
 & -\hat{A}_{gg}^{(2),\text{irr}}\left(\frac{\hat{m}_1^2}{\mu^2}\right)\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_2^2}{\mu^2}\right)-\hat{A}_{gg}^{(2),\text{irr}}\left(\frac{\hat{m}_2^2}{\mu^2}\right)\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_1^2}{\mu^2}\right) \\
 & -2\hat{A}_{gg}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}\right)\hat{\Pi}^{(2)}\left(0,\frac{\hat{m}_2^2}{\mu^2}\right)-2\hat{A}_{gg}^{(1)}\left(\frac{\hat{m}_2^2}{\mu^2}\right)\hat{\Pi}^{(2)}\left(0,\frac{\hat{m}_1^2}{\mu^2}\right) \\
 & +\hat{A}_{gg}^{(1)}\left(\frac{\hat{m}_1^2}{\mu^2}\right)\left[2\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_1^2}{\mu^2}\right)+\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_2^2}{\mu^2}\right)\right]\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_2^2}{\mu^2}\right) \\
 & +\hat{A}_{gg}^{(1)}\left(\frac{\hat{m}_2^2}{\mu^2}\right)\left[2\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_2^2}{\mu^2}\right)+\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_1^2}{\mu^2}\right)\right]\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}_1^2}{\mu^2}\right).
 \end{aligned} \tag{5.91}$$

## 5.6. The General Structure of the Massive Operator Matrix Elements

In the following, the structure of the different unrenormalized and renormalized OMEs for the genuine two-mass contributions are presented.

In the case of only one heavy quark flavor with mass  $m$  [182], the mass dependence of the unrenormalized massive operator matrix element at order  $\alpha_s^l$  is given by

$$\hat{A}_{ij}^{(l)}\left(\frac{\hat{m}^2}{\mu^2},\varepsilon,N\right) = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\frac{l\varepsilon}{2}} \hat{A}_{ij}^{(l)}(\varepsilon,N). \tag{5.92}$$

Here the OME  $\hat{A}_{ij}^{(l)}(\varepsilon,N)$  does not depend on the mass explicitly anymore. It exhibits poles in the dimensional parameter  $\varepsilon$  up to  $\varepsilon^{-l}$

$$\hat{A}_{ij}^{(l)}(\varepsilon,N) = \sum_{k=0}^{\infty} \frac{a_{ij}^{(l,k)}}{\varepsilon^{l-k}}. \tag{5.93}$$

Adopting the notation of Ref. [182] one can define

$$a^{(l,l)} \equiv a^{(l)}, \quad a^{(l,l+1)} \equiv \bar{a}^{(l)}. \tag{5.94}$$

The unrenormalized operator matrix elements with two massive fermion flavors with masses  $m_1 \neq m_2$  are split into the respective single-mass contributions, cf. Eqs. (5.92) and (5.93), and a part  $\hat{A}_{ij}^{(l)}\left(\frac{\hat{m}_1^2}{\mu^2},\frac{\hat{m}_2^2}{\mu^2},\varepsilon,N\right)$  depending on both masses

$$\hat{A}_{ij}^{(l)}\left(\frac{\hat{m}_1^2}{\mu^2},\frac{\hat{m}_2^2}{\mu^2},\varepsilon,N\right) = \left[\left(\frac{\hat{m}_1^2}{\mu^2}\right)^{\frac{l\varepsilon}{2}} + \left(\frac{\hat{m}_2^2}{\mu^2}\right)^{\frac{l\varepsilon}{2}}\right] \hat{A}_{ij}^{(l)}(\varepsilon,N) + \hat{A}_{ij}^{(l)}\left(\frac{\hat{m}_1^2}{\mu^2},\frac{\hat{m}_2^2}{\mu^2},\varepsilon,N\right). \tag{5.95}$$

The two-flavor contributions  $\hat{A}_{ij}^{(l)}\left(\frac{\hat{m}_1^2}{\mu^2},\frac{\hat{m}_2^2}{\mu^2},\varepsilon,N\right)$ ,  $m_1 \neq m_2$ , to the massive OMEs do not obey a factorization relation as in Eq. (5.92) and the mass dependence is pulled into the coefficients of the Laurent expansion

$$\hat{A}_{ij}^{(l)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}, \varepsilon, N\right) = \sum_{k=0}^{\infty} \frac{\tilde{a}_{ij}^{(l,k)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right)}{\varepsilon^{l-k}}. \quad (5.96)$$

Analogously to Eq. (5.94) one can define

$$\tilde{a}^{(l,l)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right) \equiv \tilde{a}^{(l)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right). \quad (5.97)$$

In the following,  $a^{(l,k)}$ ,  $a^{(l)}$ ,  $\bar{a}^{(l)}$  without argument will denote the single mass-quantities corresponding to the definitions in Eqs. (5.93) and (5.94), while  $\tilde{a}^{(l,l)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}\right)$  refers to the two-mass contribution. From Eq. (5.64) it is obvious that the renormalization of the 3-loop OMEs requires the knowledge of the one-loop OMEs  $A_{ij}^{(1)}(m_1, m_2)$  up to  $\mathcal{O}(\varepsilon^2)$  and the two-loop OMEs  $A_{ij}^{(2)}(m_1, m_2)$  up to  $\mathcal{O}(\varepsilon)$ . Up to  $\mathcal{O}(\alpha_s^2)$ , these two mass quantities can be traced back to the corresponding single-mass quantities by Eqs. (5.81-5.82) and in Eqs. (5.83-5.85).

It is technically advantageous to perform the renormalization on the complete two-flavor OMEs  $\hat{A}_{ij}^{(l)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}, \varepsilon, N\right)$ . For brevity and to avoid redundancy with respect to [182] the renormalization formulas for the two-mass contribution  $\hat{A}_{ij}^{(l)}\left(\frac{\hat{m}_1^2}{\mu^2}, \frac{\hat{m}_2^2}{\mu^2}, \varepsilon, N\right)$  only are presented. These quantities are obtained by subtracting the respective single-mass contributions [176, 182].

The analytic expressions for the respective single mass contributions and renormalization constants to two-loop order, which appear in subsequent relations, have been given in Refs. [145, 146, 182, 185, 186] and references therein.

### $A_{qq,Q}^{\text{NS}}$

The lowest non-trivial flavor non-singlet (NS) contribution is of  $\mathcal{O}(a_s^2)$ ,

$$A_{qq,Q}^{\text{NS}} = 1 + a_s^2 A_{qq,Q}^{(2),\text{NS}} + a_s^3 A_{qq,Q}^{(3),\text{NS}} + \mathcal{O}(a_s^4). \quad (5.98)$$

Starting from  $\mathcal{O}(a_s^3)$  it exhibits a non-trivial two-mass contribution

$$\tilde{A}_{qq,Q}^{\text{NS}} = 1 + a_s^3 \tilde{A}_{qq,Q}^{(3),\text{NS}} + \mathcal{O}(a_s^4). \quad (5.99)$$

The renormalized two-mass OME in the MOM-scheme is obtained from the bare quantities combining Eqs. (5.41) and (5.64). It is given by

$$\begin{aligned} A_{qq,Q}^{(3),\text{NS},\text{MOM}}(N_F + 2) &= \hat{A}_{qq,Q}^{(3),\text{NS},\text{MOM}} + Z_{qq}^{-1,(3),\text{NS}}(N_F + 2) - Z_{qq}^{-1,(3),\text{NS}}(N_F) \\ &\quad + Z_{qq}^{-1,(1),\text{NS}}(N_F + 2) \hat{A}_{qq,Q}^{(2),\text{NS},\text{MOM}} + \left[ \hat{A}_{qq,Q}^{(2),\text{NS},\text{MOM}} \right. \\ &\quad \left. + Z_{qq}^{-1,(2),\text{NS}}(N_F + 2) - Z_{qq}^{-1,(2),\text{NS}}(N_F) \right] \Gamma_{qq}^{-1,(1)}(N_F). \end{aligned} \quad (5.100)$$

After a finite renormalization to the  $\overline{\text{MS}}$ -scheme and the subtraction of the single-mass contributions one obtains the pole-structure of the two-flavor piece by

$$\hat{A}_{qq,Q}^{(3),\text{NS}} = -\frac{16}{3\varepsilon^3} \gamma_{qq}^{(0)} \beta_{0,Q}^2 + \frac{1}{\varepsilon^2} \left[ -\frac{4}{3} \beta_{0,Q} \gamma_{qq}^{\text{NS},(1)} - 4\gamma_{qq}^{(0)} \beta_{0,Q}^2 (L_1 + L_2) \right]$$



$$\begin{aligned}
 & + \frac{1}{\varepsilon} \left[ -\beta_{0,Q} \hat{\gamma}_{qq}^{\text{NS},(1)} (L_1 + L_2) - 2\gamma_{qq}^{(0)} \beta_{0,Q}^2 (L_1^2 + L_1 L_2 + L_2^2) \right. \\
 & \left. - 8a_{qq}^{\text{NS},(2)} \beta_{0,Q} + \frac{2}{3} \gamma_{qq}^{(2),\text{NS},N_F^2} \right] + \tilde{a}_{qq,Q}^{(3),\text{NS}} (m_1^2, m_2^2, \mu^2) , \tag{5.101}
 \end{aligned}$$

with

$$L_1 = \ln \left( \frac{m_1^2}{\mu^2} \right) , \quad L_2 = \ln \left( \frac{m_2^2}{\mu^2} \right) . \tag{5.102}$$

The renormalized expression in the  $\overline{\text{MS}}$ -scheme is given by

$$\begin{aligned}
 \tilde{A}_{qq,Q}^{(3),\overline{\text{MS}},\text{NS}} & = \gamma_{qq}^{(0)} \beta_{0,Q}^2 \left( \frac{2}{3} L_1^3 + \frac{2}{3} L_2^3 + \frac{1}{2} L_1^2 L_2 + \frac{1}{2} L_2^2 L_1 \right) + \frac{1}{2} \beta_{0,Q} \hat{\gamma}_{qq}^{\text{NS},(1)} (L_1^2 + L_2^2) \\
 & + \left\{ 4a_{qq}^{\text{NS},(2)} \beta_{0,Q} + \frac{1}{2} \beta_{0,Q}^2 \gamma_{qq}^{(0)} \zeta_2 \right\} (L_1 + L_2) + 8\bar{a}_{qq}^{\text{NS},(2)} \beta_{0,Q} \\
 & + \tilde{a}_{qq,Q}^{(3),\text{NS}} (m_1^2, m_2^2, \mu^2) . \tag{5.103}
 \end{aligned}$$

For  $N = 1$  the OME vanishes due to fermion number conservation; this applies both for the anomalous dimensions  $\gamma_{qq}^{(l)}$  and the expansion coefficients of the OMEs  $a_{qq}^{\text{NS},(2)}$ ,  $\bar{a}_{qq}^{\text{NS},(2)}$  and  $\tilde{a}_{qq,Q}^{(3),\text{NS}}$ .

### $A_{Qq}^{\text{PS}}$

Depending on whether the operator couples to a heavy or a light fermion, there are two pure-singlet contributions[182]

$$A_{Qq}^{\text{PS}} = a_s^2 A_{Qq}^{(2),\text{PS}} + a_s^3 A_{Qq}^{(3),\text{PS}} + \mathcal{O}(a_s^4) , \tag{5.104}$$

$$A_{qq,Q}^{\text{PS}} = a_s^3 A_{qq,Q}^{(3),\text{PS}} + \mathcal{O}(a_s^4) . \tag{5.105}$$

Up to  $\mathcal{O}(a_s^3)$  only the OME  $A_{Qq}^{\text{PS}}$  contains a generic two-mass contribution, since  $A_{qq,Q}^{\text{PS}}$  emerges only at  $\mathcal{O}(a_s^3)$  and contains one internal massless fermion line. One has

$$\tilde{A}_{Qq}^{\text{PS}} = a_s^3 \tilde{A}_{Qq}^{(3),\text{PS}} + \mathcal{O}(a_s^4) . \tag{5.106}$$

The combined renormalization relation at third order is given by

$$\begin{aligned}
 A_{Qq}^{(3),\text{PS},\text{MOM}} + A_{qq,Q}^{(3),\text{PS},\text{MOM}} & = \hat{A}_{Qq}^{(3),\text{PS},\text{MOM}} + \hat{A}_{qq,Q}^{(3),\text{PS},\text{MOM}} + Z_{qq}^{-1,(3),\text{PS}} (N_F + 2) \\
 & - Z_{qq}^{-1,(3),\text{PS}} (N_F) + Z_{qq}^{-1,(1)} (N_F + 2) \hat{A}_{Qq}^{(2),\text{PS},\text{MOM}} + Z_{qq}^{-1,(1)} (N_F + 2) \hat{A}_{qq,Q}^{(2),\text{MOM}} \\
 & + \left[ \hat{A}_{Qq}^{(1),\text{MOM}} + Z_{qq}^{-1,(1)} (N_F + 2) - Z_{qq}^{-1,(1)} (N_F) \right] \Gamma_{qq}^{-1,(2)} (N_F) + \left[ \hat{A}_{Qq}^{(2),\text{PS},\text{MOM}} \right. \\
 & + Z_{qq}^{-1,(2),\text{PS}} (N_F + 2) - Z_{qq}^{-1,(2),\text{PS}} (N_F) \left. \right] \Gamma_{qq}^{-1,(1)} (N_F) + \left[ \hat{A}_{Qq}^{(2),\text{MOM}} + Z_{qq}^{-1,(2)} (N_F + 2) \right. \\
 & \left. - Z_{qq}^{-1,(2)} (N_F) + Z_{qq}^{-1,(1)} (N_F + 2) A_{Qq}^{(1),\text{MOM}} + Z_{qq}^{-1,(1)} (N_F + 2) A_{qq,Q}^{(1),\text{MOM}} \right] \Gamma_{qq}^{-1,(1)} (N_F) . \tag{5.107}
 \end{aligned}$$

This yields the generic pole structure for the PS two-mass contribution

$$\hat{\hat{A}}_{Qq}^{(3),\text{PS}} = \frac{8}{3\varepsilon^3} \gamma_{gg}^{(0)} \hat{\gamma}_{qq}^{(0)} \beta_{0,Q} + \frac{1}{\varepsilon^2} \left[ 2\gamma_{gg}^{(0)} \hat{\gamma}_{qq}^{(0)} \beta_{0,Q} (L_1 + L_2) + \frac{1}{6} \hat{\gamma}_{qq}^{(0)} \hat{\gamma}_{gg}^{(1)} - \frac{4}{3} \beta_{0,Q} \hat{\gamma}_{qq}^{\text{PS},(1)} \right]$$

## 5. Renormalization of the Massive Operator Matrix Elements in the Two-Mass Case

$$\begin{aligned}
& + \frac{1}{\varepsilon} \left[ \gamma_{gg}^{(0)} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} (L_1^2 + L_1 L_2 + L_2^2) + \left\{ \frac{1}{8} \hat{\gamma}_{gg}^{(0)} \hat{\gamma}_{gg}^{(1)} - \beta_{0,Q} \hat{\gamma}_{qq}^{\text{PS},(1)} \right\} (L_1 + L_2) \right. \\
& \left. + \frac{2}{3} \hat{\gamma}_{qq}^{(2),\text{PS},N_F^2} - 8a_{Qq}^{(2),\text{PS}} \beta_{0,Q} + \hat{\gamma}_{gg}^{(0)} a_{gg}^{(2)} \right] + \tilde{a}_{Qq}^{(3),\text{PS}} (m_1^2, m_2^2, \mu^2) . \quad (5.108)
\end{aligned}$$

In the  $\overline{\text{MS}}$ -scheme one obtains the renormalized expression by

$$\begin{aligned}
\tilde{A}_{Qq}^{(3),\overline{\text{MS}},\text{PS}} &= -\gamma_{gg}^{(0)} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \left( \frac{1}{4} L_1^2 L_2 + \frac{1}{4} L_2^2 L_1 + \frac{1}{3} L_1^3 + \frac{1}{3} L_2^3 \right) \\
&+ \frac{1}{2} \left\{ -\frac{1}{8} \hat{\gamma}_{gg}^{(0)} \hat{\gamma}_{gg}^{(1)} + \beta_{0,Q} \hat{\gamma}_{qq}^{\text{PS},(1)} \right\} (L_2^2 + L_1^2) \\
&+ \left\{ 4a_{Qq}^{(2),\text{PS}} \beta_{0,Q} - \frac{1}{2} \hat{\gamma}_{gg}^{(0)} a_{gg}^{(2)} - \frac{1}{4} \beta_{0,Q} \zeta_2 \gamma_{gg}^{(0)} \hat{\gamma}_{gg}^{(0)} \right\} (L_1 + L_2) \\
&+ 8\bar{a}_{Qq}^{(2),\text{PS}} \beta_{0,Q} - \hat{\gamma}_{gg}^{(0)} \bar{a}_{gg}^{(2)} + \tilde{a}_{Qq}^{(3),\text{PS}} (m_1^2, m_2^2, \mu^2) . \quad (5.109)
\end{aligned}$$

### $A_{Qg}$

Like in the PS case, there are two different contributions to the OME  $A_{Qg}$

$$A_{Qg} = a_s A_{Qg}^{(1)} + a_s^2 A_{Qg}^{(2)} + a_s^3 A_{Qg}^{(3)} + \mathcal{O}(a_s^4) . \quad (5.110)$$

$$A_{qq,Q} = a_s^3 A_{qq,Q}^{(3)} + \mathcal{O}(a_s^4) \quad (5.111)$$

depending whether the operator couples to a light or heavy quark. Of these OMEs only  $A_{Qg}$  contains two-flavor contributions starting from  $\mathcal{O}(a_s^2)$

$$\tilde{A}_{Qg} = a_s^2 \tilde{A}_{Qg}^{(2)} + a_s^3 \tilde{A}_{Qg}^{(3)} + \mathcal{O}(a_s^4) . \quad (5.112)$$

In Eq. (5.112) the  $\mathcal{O}(a_s^2)$  contribution consists of one-particle reducible diagrams only, see Eq. (5.84). As a consequence the flavor dependence factorizes in the  $\mathcal{O}(a_s^2)$  terms.

The renormalized MOM-scheme two-loop contribution is obtained by

$$\begin{aligned}
A_{Qg}^{(2),\text{MOM}} &= \hat{A}_{Qg}^{(2),\text{MOM}} + Z_{qq}^{-1,(2)} (N_F + 2) - Z_{qq}^{-1,(2)} (N_F) + Z_{qq}^{-1,(1)} (N_F + 2) \hat{A}_{gg,Q}^{(1),\text{MOM}} \\
&+ Z_{qq}^{-1,(1)} (N_F + 2) \hat{A}_{Qg}^{(1),\text{MOM}} + \left[ \hat{A}_{Qg}^{(1),\text{MOM}} + Z_{qq}^{-1,(1)} (N_F + 2) \right. \\
&\left. - Z_{qq}^{-1,(1)} (N_F) \right] \Gamma_{gg}^{-1,(1)} (N_F) . \quad (5.113)
\end{aligned}$$

The unrenormalized terms are given by

$$\begin{aligned}
\hat{A}_{Qg}^{(2)} &= -\frac{2}{\varepsilon^2} \beta_{0,Q} \hat{\gamma}_{gg}^{(0)} - \frac{1}{\varepsilon} \beta_{0,Q} \hat{\gamma}_{gg}^{(0)} (L_1 + L_2) + \tilde{a}_{Qg}^{(2)} \\
&+ \varepsilon \bar{\tilde{a}}_{Qg}^{(2)} . \quad (5.114)
\end{aligned}$$

The coefficients  $\tilde{a}_{Qg}^{(2)}$  and  $\bar{\tilde{a}}_{Qg}^{(2)}$  are read off from Eq. (5.84)

$$\tilde{a}_{Qg}^{(2)} = -\frac{1}{2} \beta_{0,Q} \hat{\gamma}_{gg}^{(0)} \left\{ \frac{1}{2} (L_1 + L_2)^2 + \zeta_2 \right\} , \quad (5.115)$$

$$\bar{\tilde{a}}_{Qg}^{(2)} = \frac{1}{2} \beta_{0,Q} \hat{\gamma}_{gg}^{(0)} \left\{ -\frac{1}{12} (L_1 + L_2)^3 - \frac{1}{2} \zeta_2 (L_1 + L_2) - \frac{1}{3} \zeta_3 \right\} . \quad (5.116)$$

The renormalized expression at 2 loops then reads

$$\begin{aligned}\tilde{A}_{Qg}^{(2),\overline{\text{MS}}} &= \frac{1}{4}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)}(L_1^2 + L_2^2) + \frac{1}{2}\zeta_2\beta_{0,Q}\hat{\gamma}_{qg}^{(0)} + \tilde{a}_{Qg}^{(2)} \\ &= -\frac{1}{2}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)}L_1L_2\end{aligned}\quad (5.117)$$

The renormalized 3-loop OMEs in the MOM-scheme are obtained from the charge- and mass-renormalized OMEs by

$$\begin{aligned}A_{Qg}^{(3),\text{MOM}} + A_{qg,Q}^{(3),\text{MOM}} &= \hat{A}_{Qg}^{(3),\text{MOM}} + \hat{A}_{qg,Q}^{(3),\text{MOM}} + Z_{qg}^{-1,(3)}(N_F + 2) - Z_{qg}^{-1,(3)}(N_F) \\ &+ Z_{qg}^{-1,(2)}(N_F + 2)\hat{A}_{qg,Q}^{(1),\text{MOM}} + Z_{qg}^{-1,(1)}(N_F + 2)\hat{A}_{qg,Q}^{(2),\text{MOM}} + Z_{qg}^{-1,(2)}(N_F + 2)\hat{A}_{Qg}^{(1),\text{MOM}} \\ &+ Z_{qg}^{-1,(1)}(N_F + 2)\hat{A}_{Qg}^{(2),\text{MOM}} + \left[\hat{A}_{Qg}^{(1),\text{MOM}} + Z_{qg}^{-1,(1)}(N_F + 2) \right. \\ &- \left. Z_{qg}^{-1,(1)}(N_F)\right]\Gamma_{gg}^{-1,(2)}(N_F) + \left[\hat{A}_{Qg}^{(2),\text{MOM}} + Z_{qg}^{-1,(2)}(N_F + 2) - Z_{qg}^{-1,(2)}(N_F) \right. \\ &+ \left. Z_{qg}^{-1,(1)}(N_F + 2)A_{Qg}^{(1),\text{MOM}} + Z_{qg}^{-1,(1)}(N_F + 2)A_{qg,Q}^{(1),\text{MOM}}\right]\Gamma_{gg}^{-1,(1)}(N_F) \\ &+ \left[\hat{A}_{Qg}^{(2),\text{PS},\text{MOM}} + Z_{qg}^{-1,(2),\text{PS}}(N_F + 2) - Z_{qg}^{-1,(2),\text{PS}}(N_F)\right]\Gamma_{qg}^{-1,(1)}(N_F) \\ &+ \left[\hat{A}_{qg,Q}^{(2),\text{NS},\text{MOM}} + Z_{qg}^{-1,(2),\text{NS}}(N_F + 2) - Z_{qg}^{-1,(2),\text{NS}}(N_F)\right]\Gamma_{qg}^{-1,(1)}(N_F).\end{aligned}\quad (5.118)$$

It is explicitly given by

$$\begin{aligned}\hat{A}_{Qg}^{(3)} &= \frac{1}{\varepsilon^3}\left[\frac{14}{3}\beta_{0,Q}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)} - \frac{4}{3}\hat{\gamma}_{qg}^{(0)}\gamma_{qg}^{(0)}\beta_{0,Q} + \frac{7}{3}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)}\gamma_{gg}^{(0)} + 12\beta_{0,Q}^2\hat{\gamma}_{qg}^{(0)} + \frac{1}{12}\gamma_{qg}^{(0)}\left(\hat{\gamma}_{qg}^{(0)}\right)^2\right] \\ &+ \frac{1}{\varepsilon^2}\left\{\frac{1}{16}\gamma_{qg}^{(0)}\left(\hat{\gamma}_{qg}^{(0)}\right)^2 + 9\beta_{0,Q}^2\hat{\gamma}_{qg}^{(0)} + \frac{7}{2}\beta_{0,Q}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)} - \hat{\gamma}_{qg}^{(0)}\gamma_{qg}^{(0)}\beta_{0,Q} + \frac{7}{4}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)}\gamma_{gg}^{(0)}\right\} \\ &\times (L_1 + L_2) + \frac{1}{12}\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{qg}^{\text{PS},(1)} + \frac{1}{12}\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{qg}^{\text{NS},(1)} - \frac{5}{3}\beta_{0,Q}\hat{\gamma}_{qg}^{(1)} + \frac{1}{6}\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{gg}^{(1)} - \frac{1}{3}\hat{\gamma}_{qg}^{(0)}\beta_{1,Q} \\ &+ 5\hat{\gamma}_{qg}^{(0)}\beta_{0,Q}\delta m_1^{(-1)}\left] + \frac{1}{\varepsilon}\left\{\frac{1}{16}\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{qg}^{\text{NS},(1)} + \frac{15}{4}\hat{\gamma}_{qg}^{(0)}\beta_{0,Q}\delta m_1^{(-1)} + \frac{1}{16}\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{qg}^{\text{PS},(1)} - \frac{5}{4}\beta_{0,Q}\hat{\gamma}_{qg}^{(1)} \right. \\ &+ \left. \frac{1}{8}\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{gg}^{(1)} - \frac{1}{4}\hat{\gamma}_{qg}^{(0)}\beta_{1,Q}\right\}(L_1 + L_2) + \left\{\frac{13}{8}\beta_{0,Q}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)} + \frac{13}{16}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)}\gamma_{gg}^{(0)} + \frac{15}{4}\beta_{0,Q}^2\hat{\gamma}_{qg}^{(0)} \right. \\ &+ \left. \frac{3}{64}\gamma_{qg}^{(0)}\left(\hat{\gamma}_{qg}^{(0)}\right)^2 - \frac{1}{2}\hat{\gamma}_{qg}^{(0)}\gamma_{qg}^{(0)}\beta_{0,Q}\right\}(L_1^2 + L_2^2) + \left\{-\frac{1}{2}\hat{\gamma}_{qg}^{(0)}\gamma_{qg}^{(0)}\beta_{0,Q} + 2\beta_{0,Q}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)} + 6\beta_{0,Q}^2\hat{\gamma}_{qg}^{(0)} \right. \\ &+ \left. \beta_{0,Q}\hat{\gamma}_{qg}^{(0)}\gamma_{gg}^{(0)}\right\}L_1L_2 + \frac{2}{3}\gamma_{qg}^{(2),N_F^2} - 8\beta_{0,Q}a_{Qg}^{(2)} - \frac{1}{32}\left(\hat{\gamma}_{qg}^{(0)}\right)^2\zeta_2\gamma_{qg}^{(0)} + \hat{\gamma}_{qg}^{(0)}a_{qg,Q}^{(2)} - \hat{\gamma}_{qg}^{(0)}\tilde{\delta}m_2^{(-1)} \\ &+ \frac{9}{2}\hat{\gamma}_{qg}^{(0)}\zeta_2\beta_{0,Q}^2 + \frac{1}{8}\beta_{0,Q}\zeta_2\hat{\gamma}_{qg}^{(0)}\gamma_{gg}^{(0)} + \frac{1}{4}\hat{\gamma}_{qg}^{(0)}\zeta_2\beta_{0,Q}\beta_0 + 4\delta m_1^{(0)}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)}\left] \right. \\ &+ \tilde{a}_{Qg}^{(3)}(m_1^2, m_2^2, \mu^2).\end{aligned}\quad (5.119)$$

For the renormalized operator matrix element in the  $\overline{\text{MS}}$  scheme one finally obtains,

$$\tilde{A}_{Qg}^{(3),\overline{\text{MS}}} = \left\{-\frac{9}{8}\beta_{0,Q}^2\hat{\gamma}_{qg}^{(0)} - \frac{7}{384}\gamma_{qg}^{(0)}\left(\hat{\gamma}_{qg}^{(0)}\right)^2 + \frac{1}{6}\hat{\gamma}_{qg}^{(0)}\gamma_{qg}^{(0)}\beta_{0,Q} - \frac{25}{96}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)}\gamma_{gg}^{(0)} - \frac{25}{48}\beta_{0,Q}\beta_{0,Q}\hat{\gamma}_{qg}^{(0)}\right\}$$

5. Renormalization of the Massive Operator Matrix Elements in the Two-Mass Case

$$\begin{aligned}
& \times (L_1^3 + L_2^3) + \left\{ \frac{1}{8} \hat{\gamma}_{gg}^{(0)} \gamma_{qq}^{(0)} \beta_{0,Q} - \frac{1}{2} \beta_0 \beta_{0,Q} \hat{\gamma}_{gg}^{(0)} - \frac{1}{4} \beta_{0,Q} \hat{\gamma}_{gg}^{(0)} \gamma_{gg}^{(0)} - \frac{3}{2} \beta_{0,Q}^2 \hat{\gamma}_{gg}^{(0)} \right\} \\
& \times (L_1^2 L_2 + L_2^2 L_1) + \left\{ -\frac{1}{64} \hat{\gamma}_{gg}^{(0)} \hat{\gamma}_{qq}^{\text{PS},(1)} - \frac{1}{64} \hat{\gamma}_{gg}^{(0)} \hat{\gamma}_{qq}^{\text{NS},(1)} + \frac{9}{16} \beta_{0,Q} \hat{\gamma}_{gg}^{(1)} - \frac{1}{16} \hat{\gamma}_{gg}^{(0)} \hat{\gamma}_{gg}^{(1)} \right. \\
& \left. - \frac{29}{16} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \delta m_1^{(-1)} + \frac{1}{16} \hat{\gamma}_{gg}^{(0)} \beta_{1,Q} \right\} (L_1^2 + L_2^2) - 2L_1 L_2 \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \delta m_1^{(-1)} + \left\{ \frac{3}{4} \hat{\gamma}_{gg}^{(0)} \tilde{\delta} m_2^{(-1)} \right. \\
& \left. + \frac{1}{128} \left( \hat{\gamma}_{gg}^{(0)} \right)^2 \zeta_2 \gamma_{gg}^{(0)} + \frac{1}{8} \hat{\gamma}_{gg}^{(0)} \zeta_2 \beta_{0,Q} \gamma_{qq}^{(0)} - 3\delta m_1^{(0)} \beta_{0,Q} \hat{\gamma}_{gg}^{(0)} - \frac{1}{2} \hat{\gamma}_{gg}^{(0)} a_{gg,Q}^{(2)} - \frac{9}{32} \beta_{0,Q} \zeta_2 \hat{\gamma}_{gg}^{(0)} \gamma_{gg}^{(0)} \right. \\
& \left. - \frac{27}{8} \hat{\gamma}_{gg}^{(0)} \zeta_2 \beta_{0,Q}^2 - \frac{9}{16} \hat{\gamma}_{gg}^{(0)} \zeta_2 \beta_{0,Q} \beta_0 + 4\beta_{0,Q} a_{Qg}^{(2)} \right\} (L_1 + L_2) + 8\bar{a}_{Qg}^{(2)} \beta_{0,Q} - \frac{1}{32} \hat{\gamma}_{gg}^{(0)} \zeta_2 \hat{\gamma}_{qq}^{\text{PS},(1)} \\
& - \frac{1}{32} \hat{\gamma}_{gg}^{(0)} \zeta_2 \hat{\gamma}_{qq}^{\text{NS},(1)} + \frac{1}{96} \left( \hat{\gamma}_{gg}^{(0)} \right)^2 \zeta_3 \gamma_{gg}^{(0)} - \frac{3}{2} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q}^2 \zeta_3 + \frac{1}{8} \hat{\gamma}_{gg}^{(1)} \beta_{0,Q} \zeta_2 - 4\delta m_1^{(1)} \beta_{0,Q} \hat{\gamma}_{gg}^{(0)} \\
& + \frac{1}{8} \hat{\gamma}_{gg}^{(0)} \zeta_2 \beta_{1,Q} - \hat{\gamma}_{gg}^{(0)} \bar{a}_{gg,Q}^{(2)} - \frac{1}{12} \hat{\gamma}_{gg}^{(0)} \beta_0 \beta_{0,Q} \zeta_3 - \frac{1}{24} \beta_{0,Q} \zeta_3 \hat{\gamma}_{gg}^{(0)} \gamma_{gg}^{(0)} + \frac{1}{2} \hat{\gamma}_{gg}^{(0)} \left( \tilde{\delta} m_2^{1,(0)} \right. \\
& \left. + \tilde{\delta} m_2^{2,(0)} \right) - \frac{9}{8} \hat{\gamma}_{gg}^{(0)} \zeta_2 \beta_{0,Q} \delta m_1^{(-1)} + \bar{a}_{Qg}^{(3)} (m_1^2, m_2^2, \mu^2) . \tag{5.120}
\end{aligned}$$

$A_{gq,Q}$

The matrix element  $A_{gq,Q}$  contains contributions starting at  $\mathcal{O}(a_s^2)$ ,

$$A_{gq,Q} = a_s^2 A_{gq,Q}^{(2)} + a_s^3 A_{gq,Q}^{(3)} + \mathcal{O}(a_s^4) . \tag{5.121}$$

Diagrams with two different masses, however, contribute only from  $\mathcal{O}(a_s^3)$

$$\tilde{A}_{gq,Q} = a_s^3 \tilde{A}_{gq,Q}^{(3)} + \mathcal{O}(a_s^4) . \tag{5.122}$$

The renormalization in the MOM-scheme is performed using

$$\begin{aligned}
A_{gq,Q}^{(2),\text{MOM}} &= \hat{A}_{gq,Q}^{(2),\text{MOM}} + Z_{gg}^{-1,(2)} (N_F + 2) - Z_{gg}^{-1,(2)} (N_F) \\
&+ \left( \hat{A}_{gg,Q}^{(1),\text{MOM}} + Z_{gg}^{-1,(1)} (N_F + 2) - Z_{gg}^{-1,(1)} (N_F) \right) \Gamma_{gg}^{-1,(1)} , \tag{5.123}
\end{aligned}$$

$$\begin{aligned}
A_{gq,Q}^{(3),\text{MOM}} &= \hat{A}_{gq,Q}^{(3),\text{MOM}} + Z_{gg}^{-1,(3)} (N_F + 2) - Z_{gg}^{-1,(3)} (N_F) + Z_{gg}^{-1,(1)} (N_F + 2) \hat{A}_{gq,Q}^{(2),\text{MOM}} \\
&+ Z_{gg}^{-1,(1)} (N_F + 2) \hat{A}_{qq}^{(2),\text{MOM}} + \left[ \hat{A}_{gg,Q}^{(1),\text{MOM}} + Z_{gg}^{-1,(1)} (N_F + 2) \right. \\
&\left. - Z_{gg}^{-1,(1)} (N_F) \right] \Gamma_{qq}^{-1,(2)} (N_F) + \left[ \hat{A}_{gq,Q}^{(2),\text{MOM}} + Z_{gg}^{-1,(2)} (N_F + 2) \right. \\
&\left. - Z_{gg}^{-1,(2)} (N_F) \right] \Gamma_{qq}^{-1,(1)} (N_F) + \left[ \hat{A}_{gq,Q}^{(2),\text{MOM}} + Z_{gg}^{-1,(2)} (N_F + 2) \right. \\
&\left. - Z_{gg}^{-1,(2)} (N_F) + Z_{gg}^{-1,(1)} (N_F + 2) \hat{A}_{gq,Q}^{(1),\text{MOM}} \right. \\
&\left. + Z_{gg}^{-1,(1)} (N_F + 2) \hat{A}_{Qg}^{(1),\text{MOM}} \right] \Gamma_{gg}^{-1,(1)} (N_F) . \tag{5.124}
\end{aligned}$$

Applying Eq. (5.124) yields the unrenormalized expression

$$\begin{aligned}
\hat{\hat{A}}_{gq,Q}^{(3)} &= -\frac{16}{\varepsilon^3} \gamma_{gg}^{(0)} \beta_{0,Q}^2 + \frac{1}{\varepsilon^2} \left[ -12 \gamma_{gg}^{(0)} \beta_{0,Q}^2 (L_2 + L_1) - 2 \beta_{0,Q} \hat{\gamma}_{gg}^{(1)} \right] \\
&+ \frac{1}{\varepsilon} \left[ -6 \gamma_{gg}^{(0)} \beta_{0,Q}^2 (L_2^2 + L_1 L_2 + L_1^2) - \frac{3}{2} \beta_{0,Q} \hat{\gamma}_{gg}^{(1)} (L_2 + L_1) \right]
\end{aligned}$$

$$+ \frac{2}{3} \gamma_{gq}^{(2), N_F^2} - 12 a_{gq}^{(2)} \beta_{0,Q} \left. \right] + \tilde{a}_{gq,Q}^{(3)}(m_1^2, m_2^2, \mu^2) , \quad (5.125)$$

and the renormalized operator matrix element reads

$$\begin{aligned} \tilde{A}_{gq,Q}^{(3), \overline{\text{MS}}} &= \gamma_{gq}^{(0)} \beta_{0,Q}^2 \left( 2L_2^3 + 2L_1^3 + \frac{3}{2} L_2^2 L_1 + \frac{3}{2} L_1^2 L_2 \right) + \frac{3}{4} \beta_{0,Q} \hat{\gamma}_{gq}^{(1)} (L_2^2 + L_1^2) \\ &+ \left\{ 6 a_{gq}^{(2)} \beta_{0,Q} + \frac{3}{2} \gamma_{gq}^{(0)} \beta_{0,Q}^2 \zeta_2 \right\} (L_2 + L_1) + 12 \bar{a}_{gq}^{(2)} \beta_{0,Q} + \tilde{a}_{gq,Q}^{(3)}(m_1^2, m_2^2, \mu^2) . \end{aligned} \quad (5.126)$$

$A_{gg,Q}$

Finally, the matrix element  $A_{gg,Q}$  obeys the expansion

$$A_{gg,Q} = 1 + a_s A_{gg,Q}^{(1)} + a_s^2 A_{gg,Q}^{(2)} + a_s^3 A_{gg,Q}^{(3)} + \mathcal{O}(a_s^4) , \quad (5.127)$$

with two-mass contributions starting at  $\mathcal{O}(a_s^2)$ ,

$$\tilde{A}_{gg,Q} = a_s^2 \tilde{A}_{gg,Q}^{(2)} + a_s^3 \tilde{A}_{gg,Q}^{(3)} + \mathcal{O}(a_s^4) . \quad (5.128)$$

The renormalization formulae in the MOM-scheme read

$$\begin{aligned} A_{gq,Q}^{(2), \text{MOM}} &= \hat{A}_{gq,Q}^{(2), \text{MOM}} + Z_{gg}^{-1, (2)}(N_F + 2) - Z_{gg}^{-1, (2)}(N_F) \\ &+ Z_{gq}^{-1, (1)}(N_F + 2) \hat{A}_{gq,Q}^{(1), \text{MOM}} + Z_{gq}^{-1, (1)}(N_F + 2) \hat{A}_{Qg}^{(1), \text{MOM}} \\ &+ \left[ \hat{A}_{gq,Q}^{(1), \text{MOM}} + Z_{gg}^{-1, (1)}(N_F + 2) - Z_{gg}^{-1, (1)}(N_F) \right] \Gamma_{gg}^{-1, (1)}(N_F) , \quad (5.129) \\ A_{gg,Q}^{(3), \text{MOM}} &= \hat{A}_{gg,Q}^{(3), \text{MOM}} + Z_{gg}^{-1, (3)}(N_F + 2) - Z_{gg}^{-1, (3)}(N_F) + Z_{gg}^{-1, (2)}(N_F + 2) \hat{A}_{gg,Q}^{(1), \text{MOM}} \\ &+ Z_{gg}^{-1, (1)}(N_F + 2) \hat{A}_{gg,Q}^{(2), \text{MOM}} + Z_{gq}^{-1, (2)}(N_F + 2) \hat{A}_{Qg}^{(1), \text{MOM}} \\ &+ Z_{gq}^{-1, (1)}(N_F + 2) \hat{A}_{Qg}^{(2), \text{MOM}} + \left[ \hat{A}_{gg,Q}^{(1), \text{MOM}} + Z_{gg}^{-1, (1)}(N_F + 2) \right. \\ &- \left. Z_{gg}^{-1, (1)}(N_F) \right] \Gamma_{gg}^{-1, (2)}(N_F) + \left[ \hat{A}_{gg,Q}^{(2), \text{MOM}} + Z_{gg}^{-1, (2)}(N_F + 2) \right. \\ &- \left. Z_{gg}^{-1, (2)}(N_F) + Z_{gq}^{-1, (1)}(N_F + 2) A_{Qg}^{(1), \text{MOM}} \right. \\ &+ \left. Z_{gg}^{-1, (1)}(N_F + 2) A_{gg,Q}^{(1), \text{MOM}} \right] \Gamma_{gg}^{-1, (1)}(N_F) \\ &+ \left[ \hat{A}_{gq,Q}^{(2), \text{MOM}} + Z_{gq}^{-1, (2)}(N_F + 2) - Z_{gq}^{-1, (2)}(N_F) \right] \Gamma_{gq}^{-1, (1)}(N_F) . \quad (5.130) \end{aligned}$$

After subtracting all single-mass contributions we obtain the unrenormalized two-flavor contribution at 2 loops

$$\hat{\hat{A}}_{gg,Q}^{(2)} = \frac{8\beta_{0,Q}}{\varepsilon^2} + \frac{4\beta_{0,Q}^2}{\varepsilon} (L_1 + L_2) + \tilde{a}_{gg,Q} + \varepsilon \bar{\tilde{a}}_{gg,Q} \quad (5.131)$$

which are due to reducible contributions only. Therefore the  $\mathcal{O}(a_s^2)$  coefficients follow from Eq. (5.85)

$$\tilde{a}_{gg,Q}^{(2)} = \beta_{0,Q}^2 (L_2 + L_1)^2 + 2\beta_{0,Q}^2 \zeta_2 , \quad (5.132)$$

$$\bar{\tilde{a}}_{gg,Q}^{(2)} = \frac{1}{6} \beta_{0,Q}^2 (L_1 + L_2)^3 + \beta_{0,Q}^2 \zeta_2 (L_2 + L_1) + \frac{2}{3} \beta_{0,Q}^2 \zeta_3 . \quad (5.133)$$

## 5. Renormalization of the Massive Operator Matrix Elements in the Two-Mass Case

The renormalized expression reads

$$\begin{aligned}\tilde{A}_{gg,Q}^{(2),\overline{\text{MS}}} &= -\beta_{0,Q}^2 (L_1^2 + L_2^2) - 2\beta_{0,Q}^2 \zeta_2 + \tilde{a}_{gg,Q} \\ &= 2\beta_{0,Q}^2 L_1 L_2 .\end{aligned}\quad (5.134)$$

The unrenormalized 3-loop contribution from two masses reads

$$\begin{aligned}\hat{A}_{gg,Q}^{(3)} &= \frac{1}{\varepsilon^3} \left[ -\frac{5}{3} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \gamma_{gg}^{(0)} - \frac{56}{3} \beta_0 \beta_{0,Q}^2 - \frac{28}{3} \beta_{0,Q}^2 \gamma_{gg}^{(0)} - 48 \beta_{0,Q}^3 \right] + \frac{1}{\varepsilon^2} \left[ \left\{ -7\beta_{0,Q}^2 \gamma_{gg}^{(0)} \right. \right. \\ &\quad \left. \left. - 14\beta_0 \beta_{0,Q}^2 - \frac{5}{4} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \gamma_{gg}^{(0)} - 36\beta_{0,Q}^3 \right\} (L_1 + L_2) + \frac{1}{12} \hat{\gamma}_{gg}^{(0)} \hat{\gamma}_{gg}^{(1)} - \frac{7}{3} \beta_{0,Q} \hat{\gamma}_{gg}^{(1)} \right. \\ &\quad \left. + \frac{4}{3} \beta_{1,Q} \beta_{0,Q} - 20\delta m_1^{(-1)} \beta_{0,Q}^2 \right] + \frac{1}{\varepsilon} \left[ \left\{ \frac{1}{16} \hat{\gamma}_{gg}^{(0)} \hat{\gamma}_{gg}^{(1)} - 15\delta m_1^{(-1)} \beta_{0,Q}^2 - \frac{7}{4} \beta_{0,Q} \hat{\gamma}_{gg}^{(1)} \right. \right. \\ &\quad \left. \left. + \beta_{1,Q} \beta_{0,Q} \right\} (L_1 + L_2) + \left\{ -15\beta_{0,Q}^3 - \frac{11}{16} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \gamma_{gg}^{(0)} - \frac{13}{2} \beta_0 \beta_{0,Q}^2 - \frac{13}{4} \beta_{0,Q}^2 \gamma_{gg}^{(0)} \right\} \right. \\ &\quad \left. \times (L_1^2 + L_2^2) + \left\{ -4\beta_{0,Q}^2 \gamma_{gg}^{(0)} - 24\beta_{0,Q}^3 - 8\beta_0 \beta_{0,Q}^2 - \frac{1}{2} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \gamma_{gg}^{(0)} \right\} L_1 L_2 - \frac{1}{2} \beta_{0,Q}^2 \zeta_2 \gamma_{gg}^{(0)} \right. \\ &\quad \left. + \frac{2}{3} \gamma_{gg}^{(2),N_F^2} - 12\beta_{0,Q} a_{gg,Q}^{(2)} - 18\beta_{0,Q}^3 \zeta_2 + \frac{1}{8} \beta_{0,Q} \zeta_2 \gamma_{gg}^{(0)} \hat{\gamma}_{gg}^{(0)} - \beta_0 \beta_{0,Q}^2 \zeta_2 - 16\delta m_1^{(0)} \beta_{0,Q}^2 \right. \\ &\quad \left. + 4\beta_{0,Q} \tilde{\delta} m_2^{(-1)} \right] + \tilde{a}_{gg,Q}^{(3)} (m_1^2, m_2^2, \mu^2) .\end{aligned}\quad (5.135)$$

The renormalized result in the  $\overline{\text{MS}}$ -scheme is given by

$$\begin{aligned}\tilde{A}_{gg,Q}^{(3),\overline{\text{MS}}} &= \left\{ \frac{25}{24} \beta_{0,Q}^2 \gamma_{gg}^{(0)} + \frac{25}{12} \beta_0 \beta_{0,Q}^2 + \frac{9}{2} \beta_{0,Q}^3 + \frac{23}{96} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \gamma_{gg}^{(0)} \right\} (L_1^3 + L_2^3) + \left\{ \frac{1}{8} \hat{\gamma}_{gg}^{(0)} \beta_{0,Q} \gamma_{gg}^{(0)} \right. \\ &\quad \left. + \beta_{0,Q}^2 \gamma_{gg}^{(0)} + 2\beta_0 \beta_{0,Q}^2 + 6\beta_{0,Q}^3 \right\} (L_1^2 L_2 + L_2^2 L_1) + \left\{ -\frac{1}{4} \beta_{1,Q} \beta_{0,Q} + \frac{13}{16} \beta_{0,Q} \hat{\gamma}_{gg}^{(1)} \right. \\ &\quad \left. + \frac{29}{4} \delta m_1^{(-1)} \beta_{0,Q}^2 - \frac{1}{64} \hat{\gamma}_{gg}^{(0)} \hat{\gamma}_{gg}^{(1)} \right\} (L_1^2 + L_2^2) + 8L_2 L_1 \delta m_1^{(-1)} \beta_{0,Q}^2 + \left\{ \frac{9}{4} \beta_0 \beta_{0,Q}^2 \zeta_2 \right. \\ &\quad \left. + \frac{27}{2} \beta_{0,Q}^3 \zeta_2 - 3\beta_{0,Q} \tilde{\delta} m_2^{(-1)} + \frac{9}{8} \zeta_2 \beta_{0,Q}^2 \gamma_{gg}^{(0)} + 12\delta m_1^{(0)} \beta_{0,Q}^2 + \frac{3}{32} \beta_{0,Q} \zeta_2 \gamma_{gg}^{(0)} \hat{\gamma}_{gg}^{(0)} \right. \\ &\quad \left. + 6\beta_{0,Q} a_{gg,Q}^{(2)} \right\} (L_2 + L_1) - \frac{1}{32} \hat{\gamma}_{gg}^{(0)} \zeta_2 \hat{\gamma}_{gg}^{(1)} + \frac{1}{8} \beta_{0,Q} \zeta_2 \hat{\gamma}_{gg}^{(1)} + \frac{1}{3} \beta_0 \beta_{0,Q}^2 \zeta_3 + 12\beta_{0,Q} \tilde{a}_{gg,Q}^{(2)} \\ &\quad + 6\beta_{0,Q}^3 \zeta_3 + 16\delta m_1^{(1)} \beta_{0,Q}^2 + \frac{1}{6} \beta_{0,Q}^2 \zeta_3 \gamma_{gg}^{(0)} - 2\beta_{0,Q} \left( \tilde{\delta} m_2^{1,(0)} + \tilde{\delta} m_2^{2,(0)} \right) \\ &\quad + \frac{9}{2} \delta m_1^{(-1)} \beta_{0,Q}^2 \zeta_2 - \frac{1}{24} \zeta_3 \beta_{0,Q} \gamma_{gg}^{(0)} \hat{\gamma}_{gg}^{(0)} - \frac{1}{2} \zeta_2 \beta_{0,Q} \beta_{1,Q} + \tilde{a}_{gg,Q}^{(3)} (m_1^2, m_2^2, \mu^2) .\end{aligned}\quad (5.136)$$

## 6. The Variable Flavor Number Scheme at NLO

The VFNS has been introduced in Chapter 2.4. It provides matching conditions between parton distribution functions (PDFs) at  $N_F$  massless flavors and those at  $N_F+2$  flavors, at high factorization and renormalization scales  $\mu^2$ . In the past the usual approach has been to deal with a single heavy quark at a time. However, the charm and bottom quarks have rather similar masses with  $m_c^2/m_b^2 \sim 1/10$  for their pole or  $\overline{\text{MS}}$  masses at NLO and NNLO, which makes it difficult to assume  $m_c^2 \ll m_b^2$ , i.e. to consider the charm quark at  $\mu = m_b$  massless. On the other hand, it is perfectly possible to decouple both quarks simultaneously and consider their effect at high scales  $\mu \gg m_c, m_b$ . This allows to introduce heavy quark parton distribution functions, which are related to the quark-singlet ( $\Sigma$ ) and gluon ( $G$ ) distributions via the universal massive operator matrix elements (OMEs)  $A_{ij}^{(k)}(\mu^2, m_c^2, m_b^2)$ . Likewise, the flavor non-singlet, singlet and gluon distribution functions receive corresponding QCD-corrections. In this chapter we will work in the  $\overline{\text{MS}}$ -scheme in QCD, defining the heavy quark masses first in the on-shell scheme and later also transforming to the  $\overline{\text{MS}}$ -scheme. The VFNS for  $k=1$  has been discussed in Ref. [180] at NLO and at NNLO in Ref. [182] and including the two-mass effects in Ref. [202] to NNLO. In this chapter the VFNS including the two-mass effects at next-to-leading order is presented. For the next-to-next-to-leading order not all ingredients are known yet.

The parton distributions for  $N_F+2$  flavors are related to those at  $N_F$  flavors by the following relations for the *number* densities in Mellin- $N$  space

$$f_{\text{NS},i}(N_F+2, \mu^2) = \left\{ 1 + a_s^2(\mu^2) \left[ A_{qq,Q}^{\text{NS},(2)}(m_c^2) + A_{qq,Q}^{\text{NS},(2)}(m_b^2) \right] \right\} f_{\text{NS},i}(N_F, \mu^2), \quad (6.1)$$

$$\begin{aligned} \Sigma(N_F+2, \mu^2) &= \left\{ 1 + a_s^2(\mu^2) \left[ A_{qq,Q}^{\text{NS},(2)}(m_c^2) + A_{qq,Q}^{\text{PS},(2)}(m_c^2) + A_{qq,Q}^{\text{NS},(2)}(m_b^2) \right. \right. \\ &\quad \left. \left. + A_{qq,Q}^{\text{PS},(2)}(m_b^2) \right] \right\} \Sigma(N_F, \mu^2) + \left\{ a_s(\mu^2) \left[ A_{Qg}^{(1)}(m_c^2) + A_{Qg}^{(1)}(m_b^2) \right] \right. \\ &\quad \left. + a_s^2(\mu^2) \left[ A_{Qg}^{(2)}(m_c^2) + A_{Qg}^{(2)}(m_b^2) + \tilde{A}_{Qg}^{(2)}(m_c, m_b) \right] \right\} G(N_F, \mu^2), \end{aligned} \quad (6.2)$$

$$\begin{aligned} G(N_F+2, \mu^2) &= \left\{ 1 + a_s(\mu^2) \left[ A_{gg,Q}^{(1)}(m_c^2) + A_{gg,Q}^{(1)}(m_b^2) \right] + a_s^2(\mu^2) \left[ A_{gg,Q}^{(2)}(m_c^2) \right. \right. \\ &\quad \left. \left. + A_{gg,Q}^{(2)}(m_b^2) + \tilde{A}_{gg,Q}^{(2)}(m_c, m_b) \right] \right\} G(N_F, \mu^2) \\ &\quad + a_s^2(\mu^2) \left[ A_{gq,Q}^{(2)}(m_c^2) + A_{gq,Q}^{(2)}(m_b^2) \right] \Sigma(N_F, \mu^2), \end{aligned} \quad (6.3)$$

$$\begin{aligned} [f_c + f_{\bar{c}}](N_F+2, \mu^2) &= a_s^2(\mu^2) A_{Qq}^{\text{PS},(2)}(m_c) \Sigma(N_F, \mu^2) \\ &\quad + \left\{ a_s(\mu^2) A_{Qg}^{(1)}(m_c^2) + a_s^2(\mu^2) \left[ A_{Qg}^{(2)}(m_c^2) + \frac{1}{2} A_{Qg}^{(2)}(m_c, m_b) \right] \right\} G(N_F, \mu^2), \end{aligned} \quad (6.4)$$

## 6. The Variable Flavor Number Scheme at NLO

$$\begin{aligned} [f_b + f_{\bar{b}}](N_F + 2, \mu^2) &= a_s^2(\mu^2) A_{Qq}^{\text{PS},(2)}(m_b^2) \Sigma(N_F, \mu^2) \\ &+ \left\{ a_s(\mu^2) A_{Qg}^{(1)}(m_b^2) + a_s^2(\mu^2) \left[ A_{Qg}^{(2)}(m_b^2) + \frac{1}{2} A_{Qg}^{(2)}(m_c, m_b) \right] \right\} G(N_F, \mu^2). \end{aligned} \quad (6.5)$$

The quark non-singlet and singlet distributions are defined by Eqs. (2.55) and (2.56). The OMEs  $A_{ij}^{(k)}(m_i)$  and  $\tilde{A}_{ij}^{(k)}(m_c, m_b)$  depend on  $\mu^2/m_c^2$  and  $\mu^2/m_b^2$  logarithmically. Eqs. (6.1)-(6.5) describe the corresponding heavy flavor contributions at  $N_F + 2$  flavors in fixed order perturbation theory. The dependence on  $N$  of the contributing functions have been suppressed for brevity.

The flavor non-singlet distributions are not affected by two-mass terms at NLO, but first at NNLO, cf. Refs. [202, 256]. The OMEs to NLO in Equations (6.1)-(6.5) have been calculated in Refs. [179, 180, 185, 187, 260] in the equal mass case. At NNLO the OMEs have been computed for a series of moments in Ref. [182] and for a part of the OMEs for general moments  $N$  in Ref. [255–261, 346, 347] in the equal mass case. In the unequal mass case at NNLO the moments  $N = 2, 4, 6$  of all OMEs were calculated in terms of an expansion in the mass ratio in Ref. [202] and a part of the general corrections in momentum space have been computed in Refs. [1, 2, 202], see also Chapter 7.

The unequal mass corrections at NLO in Eqs. (6.1-6.5) were calculated in Ref. [202], see also Chapter 5. They are given by

$$A_{Qg}^{(2)}(m_c, m_b) = -\beta_{0,Q} \hat{\gamma}_{qg}^{(0)} \ln\left(\frac{\mu^2}{m_c^2}\right) \ln\left(\frac{\mu^2}{m_b^2}\right), \quad (6.6)$$

$$A_{gg,Q}^{(2)}(m_c, m_b) = 2\beta_{0,Q}^2 \ln\left(\frac{\mu^2}{m_c^2}\right) \ln\left(\frac{\mu^2}{m_b^2}\right), \quad (6.7)$$

where

$$\hat{\gamma}_{qg}^{(0)} = -8T_F \frac{N^2 + N + 2}{N(N+1)(N+2)}, \quad (6.8)$$

denotes the leading order splitting function for the process  $g \rightarrow q$ . The following sum rule has to be obeyed due to energy-momentum conservation, cf. Ref. [182],

$$A_{Qg}(N=2) + A_{qg,Q}(N=2) + A_{gg,Q}(N=2) = 1. \quad (6.9)$$

The OME  $A_{qg,Q}$  contributes from 3-loop order onwards only and has two heavy quark contributions only beginning at 4-loop order. The equal mass terms are already known to obey Eq. (6.9) up to  $\mathcal{O}(a_s^3)$ , cf. Ref. [182]. The NLO two mass contributions equally add up to zero for  $N = 2$ .

To illustrate the numerical effect of the NLO 2-mass terms on these distributions we consider the ratio

$$\alpha \frac{a_s^2(\mu^2) A_{ig}^{(2)}(m_c, m_b) G(N_F, \mu^2)}{\Phi(N_F + 2, \mu^2)}, \quad (6.10)$$

for  $\Phi = \Sigma, G, (\alpha = 1); [f_c + f_{\bar{c}}], [f_b + f_{\bar{b}}], (\alpha = 1/2)$ . In the case of the heavy flavor distributions, the effect is largest because it is of  $\mathcal{O}(a_s)$ . A first simple estimate yields

$$\frac{[f_c + f_{\bar{c}}]^{\text{two mass}}(N_F + 2, \mu^2)}{[f_c + f_{\bar{c}}]^{\text{all}}(N_F + 2, \mu^2)} \approx a_s \left[ \beta_{0,Q} \ln\left(\frac{\mu^2}{m_b^2}\right) + \mathcal{O}(a_s) \right], \quad (6.11)$$

and similar for  $[f_b + f_{\bar{b}}]$  by exchanging  $c \leftrightarrow b$ . Here the leading term does not depend on the parton distributions in Mellin space.



For all contributions to the OMEs but  $A_{Qg}^{(2)}$  and  $A_{gg,Q}^{(2)}$  the same relation is obtained in the  $\overline{\text{MS}}$  and on-shell scheme to  $\mathcal{O}(a_s^2)$  for mass renormalization. The transition relations for  $A_{Qg}^{(2)}$  and  $A_{gg,Q}^{(2)}$  for the single mass terms read

$$A_{Qg}^{(2),\overline{\text{MS}}}(\bar{m}) = A_{Qg}^{(2),\text{OS}}(m = \bar{m}) + 4C_F\hat{\gamma}_{qg}^{(0)} \left[ 1 + \frac{3}{4} \ln \left( \frac{\mu^2}{\bar{m}^2} \right) \right] \quad (6.12)$$

$$A_{gg,Q}^{(2),\overline{\text{MS}}}(\bar{m}) = A_{gg,Q}^{(2),\text{OS}}(m = \bar{m}) - 8C_F\beta_{0,Q} \left[ 1 + \frac{3}{4} \ln \left( \frac{\mu^2}{\bar{m}^2} \right) \right] \quad (6.13)$$

where  $\bar{m}$  denotes the  $\overline{\text{MS}}$  mass. The OMEs obey the sum rule in Eq. (6.9) in both cases because

$$\frac{\hat{\gamma}_{qg}^{(0)}(N=2)}{2} - \beta_{0,Q} = 0 \quad (6.14)$$

holds. The two-mass contributions given in Eqs. (6.6) and (6.7) at NLO are the first terms of this kind emerging and are the same in both schemes. The corresponding values of the heavy quark masses in the  $\overline{\text{MS}}$  scheme are  $\bar{m}_c = 1.24 \text{ GeV}$  and  $\bar{m}_b = 4.18 \text{ GeV}$ . The numerical integrals emerging in the present calculation have been performed using the code `AIND` [348] and the harmonic polylogarithms have been evaluated using the package `hplog` [251], cf. also Ref. [349]. The additional two-mass terms described in the present paper are of logarithmic order and are therefore of comparable size to the terms appearing in the single mass case.

The VFNS is used in many applications, cf. e.g. Ref. [350], and has even been advocated by the `pdf4lhc` recommendation, cf. Ref. [351], for use. Its correct use is also of importance for all processes at hadron colliders, such as the Tevatron and the LHC, with charm and bottom quarks in the initial state. The corresponding former parameterizations have to be changed according to the relations in Eqs. (6.2-6.5) as a consequence. Furthermore, in precision measurements of the strong coupling constant  $\alpha_s(M_Z^2)$  [352–354], the charm and bottom quark masses and the parton distribution functions, if working in the VFNS, the correct relations have to be applied.

Since in QCD fits the structure function  $F_2(x, Q^2)$  plays an important role we present the two-mass contributions to this observable for pure virtual photon exchange. It is given by

$$F_2^{(2),2\text{-mass}}(x, Q^2) = \frac{32}{3} T_F^2 a_s^2(Q^2) x \ln \left( \frac{Q^2}{m_c^2} \right) \ln \left( \frac{Q^2}{m_b^2} \right) \int_x^1 \frac{dy}{y} [y^2 + (1-y)^2] G \left( \frac{x}{y}, Q^2 \right), \quad (6.15)$$

choosing the renormalization and factorization scale  $\mu^2 = Q^2$ . We mention that for the *inclusive* heavy flavor contribution to  $F_2(x, Q^2)$  also the single heavy quark contributions of Ref. [187] have to be added working in the  $\overline{\text{MS}}$  scheme for the coupling constant renormalization, which are sometimes missing in the codes following Ref. [180]. These contributions stem from massless final states with virtual heavy quark corrections.

We add a word of caution on the use of parton distributions in the VFNS, as e.g. in the representation given in Eqs. (6.1-6.5). In assembling any observable up to a certain order in the coupling,  $a_s$ , e.g.  $l$ , the factorization theorem<sup>1</sup> leads to the cancellation of the factorization scale  $\mu_F^2 = \mu^2$ . However, the required matching is not global. 0th order Wilson coefficients match to  $l$ th order OMEs and contributions to parton distributions, 1st order Wilson coefficients to  $(l-1)$ st order OMEs and PDFs, etc. If this matching is disregarded, a corresponding  $\mu$ -dependence is implied, which in principle can be thoroughly avoided, cf. e.g. Ref. [355].

In the following numerical illustrations, we refer to the parton distribution functions at NNLO presented in Ref. [207]<sup>2</sup>, implemented in LHAPDF [298]. The flavor singlet and gluon momentum distributions for  $N_F = 3$  are depicted in Figs. 6.1 and 6.2 as functions of the Bjorken variable  $x$  and the virtuality  $Q^2$  for reference.

<sup>1</sup>See Ref. [260], Eqs. (11, 19–27).

<sup>2</sup>Very recently, a NLO variant of this fit has been presented in [356].

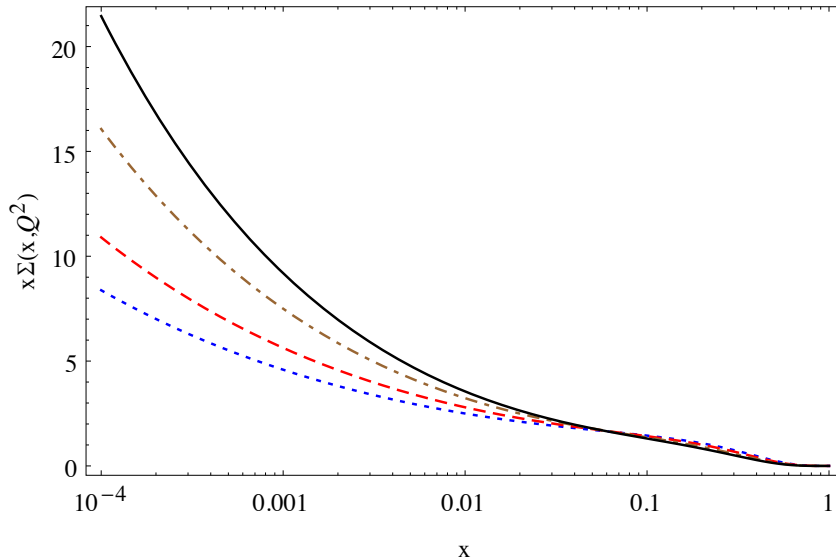


Figure 6.1.: The singlet distribution  $x\Sigma(x, Q^2)$  as a function of  $x$  and  $Q^2$  using the parton distribution functions [207]. Dotted line:  $Q^2 = 30 \text{ GeV}^2$ ; dashed line:  $Q^2 = 100 \text{ GeV}^2$ ; dash-dotted line:  $Q^2 = 1000 \text{ GeV}^2$ ; full line:  $Q^2 = 10000 \text{ GeV}^2$ .

In Figures 6.3-6.6 we show the ratios of the two-mass contributions to the total rate for the flavor singlet, gluon, charm and bottom contributions up to  $\mathcal{O}(a_s^2)$  as functions of  $x$  and  $Q^2$  according to Eqs. (6.2-6.5) in the on-mass shell scheme, setting  $\mu^2 = Q^2$ . We use the OMEs calculated in Ref. [260] in the  $\overline{\text{MS}}$  scheme for the strong coupling constant and the parton distribution functions, while the heavy quark masses are given in the on-mass shell scheme. To put the numerical effects into the perspective of later NNLO corrections we will present the illustrations choosing the NNLO values for  $a_s$ , the heavy quark masses with  $m_c = 1.59 \text{ GeV}$  and  $m_b = 4.78 \text{ GeV}$ , cf. Ref. [208, 357].

The two-mass corrections to the singlet distribution in Figure 6.3, are negative and their relative contribution varies between  $\sim 0.06\%$  at  $Q^2 = 30 \text{ GeV}^2$  to  $\sim 1.4\%$  at  $Q^2 = 10000 \text{ GeV}^2$  at  $x = 10^{-4}$  diminishing in modulus towards larger values of  $x$ .

The relative contribution of the NLO 2-mass term to the gluon distribution for  $N_F + 2$  flavors, shown in Figure 6.4, is positive and shows a slightly rising behavior in  $x$  and grows with  $\mu^2$  from values of  $\sim 0.01\%$  at  $\mu^2 = 30 \text{ GeV}^2$  to  $\sim 0.4\%$  at  $\mu^2 = 10000 \text{ GeV}^2$ . Here the positive correction balances the negative quarkonic corrections for the singlet and the heavy quark contributions.

Figures 6.5 and 6.6 show the relative two-mass corrections for the charm and bottom quark distributions. They are both negative and are slightly rising in the low  $x$  region and become larger in size for large values of  $x$ , where the distributions themselves are very small, however. For charm the largest corrections at  $x = 10^{-4}$  vary between  $\sim -0.2\%$  ( $Q^2 = 30 \text{ GeV}^2$ ) and  $\sim -3.8\%$  ( $Q^2 = 10000 \text{ GeV}^2$ ) and for bottom the corresponding values are  $\sim -2.5\%$  ( $Q^2 = 50 \text{ GeV}^2$ ) and  $\sim -4.9\%$  ( $Q^2 = 10000 \text{ GeV}^2$ ). Here we have chosen a somewhat larger lowest scale because of the heavier quark mass. Comparing the different relative corrections, the largest are those for the bottom distribution, as expected, cf. Eq. (6.11). Similar numerical results are obtained using other sets of parton distributions, as e.g. the GRV98 distributions [358].

One may sometimes resum, at least to leading order, mass logarithms into the parton densities or the coupling constant or into both. In doing this, one changes the scheme, however, from the  $\overline{\text{MS}}$ -scheme, in which the comparison of the different fitted coupling constants and/or the parton distribution functions for different analyses is performed under well defined conditions, to another new scheme. The latter now depends in many places on the chosen value of the quark masses and

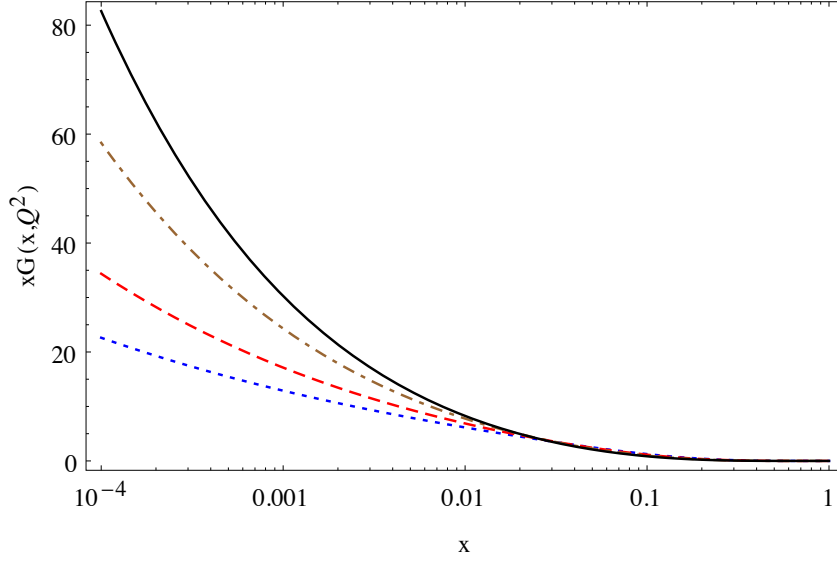


Figure 6.2.: The gluon distribution  $xG(x, Q^2)$  as a function of  $x$  and  $Q^2$  using the parton distribution functions given in Ref. [207]. Dotted line:  $Q^2 = 30 \text{ GeV}^2$ ; dashed line:  $Q^2 = 100 \text{ GeV}^2$ ; dash-dotted line:  $Q^2 = 1000 \text{ GeV}^2$ ; full line:  $Q^2 = 10\,000 \text{ GeV}^2$ .

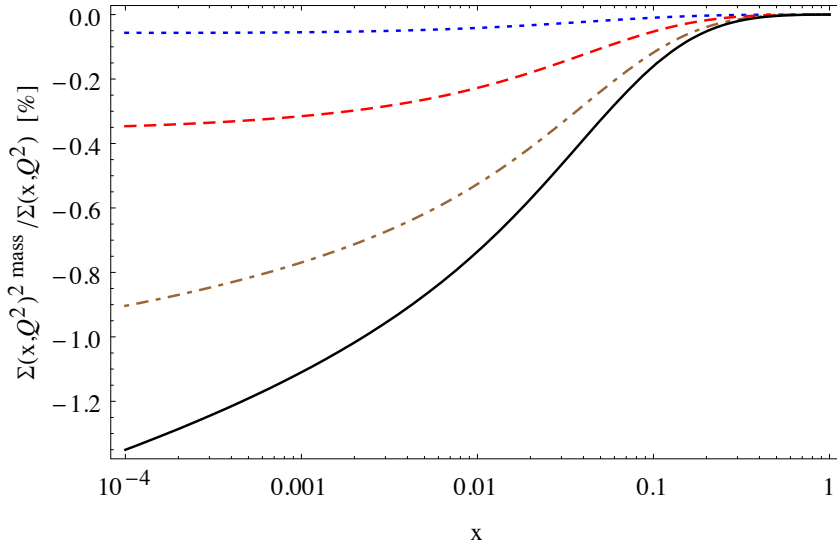


Figure 6.3.: The ratio of the two-mass contribution to the singlet distribution and the complete singlet distribution at  $\mathcal{O}(a_s^2)$ , Eq. (6.2), in %, as a function of  $x$  and  $Q^2$ , using the parton distribution functions given in Ref. [207] and  $m_c = 1.59 \text{ GeV}$  [208],  $m_b = 4.78 \text{ GeV}$  [357]. Dotted line:  $Q^2 = 30 \text{ GeV}^2$ ; dashed line:  $Q^2 = 100 \text{ GeV}^2$ ; dash-dotted line:  $Q^2 = 1000 \text{ GeV}^2$ ; full line:  $Q^2 = 10\,000 \text{ GeV}^2$ .

changes with them. As a consequence, the corresponding coupling constants and parton densities cannot be compared at all anymore. This has to be considered in precision measurements of the strong coupling constant, of the heavy quark masses, and the parton distribution functions.

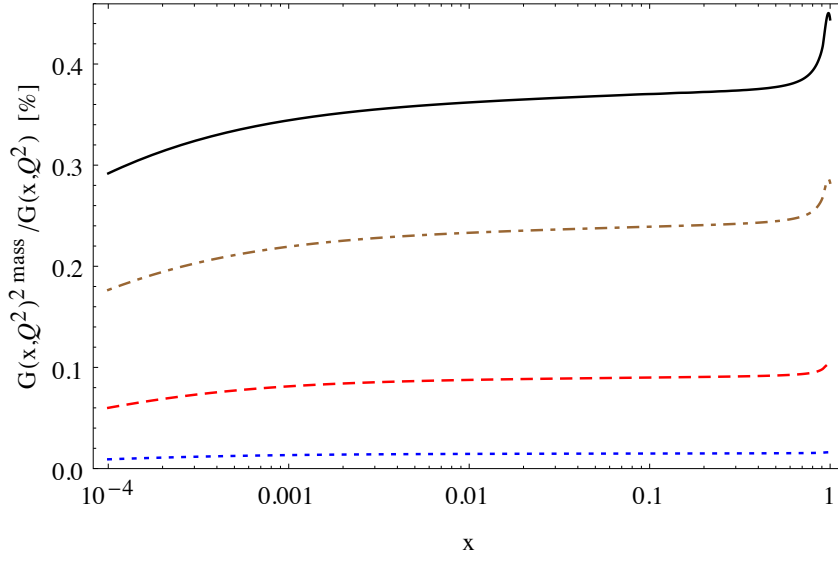


Figure 6.4.: The ratio of the two-mass contribution to the gluon distribution and the complete gluon distribution at  $\mathcal{O}(a_s^2)$ , Equation (6.3), in %, as a function of  $x$  and  $Q^2$  using the parton distribution functions given in Ref. [207] and  $m_c = 1.59$  GeV [208],  $m_b = 4.78$  GeV [357]. Dotted line:  $Q^2 = 30$  GeV<sup>2</sup>; dashed line:  $Q^2 = 100$  GeV<sup>2</sup>; dash-dotted line:  $Q^2 = 1000$  GeV<sup>2</sup>; full line:  $Q^2 = 10\,000$  GeV<sup>2</sup>.

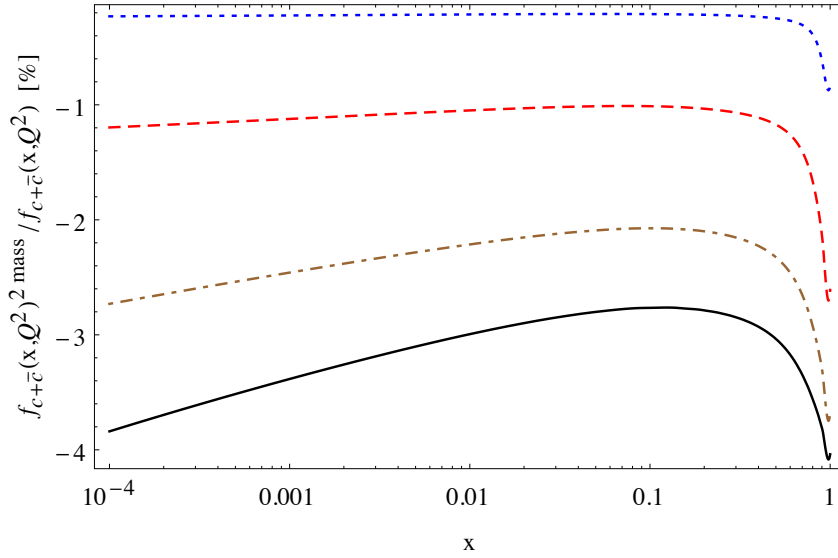


Figure 6.5.: The ratio of the two-mass contribution to the charm distribution and the complete charm distribution at  $\mathcal{O}(a_s^2)$ , Eq. (6.4), as a function of  $x$  and  $Q^2$  using the parton distribution functions given in Ref. [207] and  $m_c = 1.59$  GeV [208],  $m_b = 4.78$  GeV [357]. Dotted line:  $Q^2 = 30$  GeV<sup>2</sup>; dashed line:  $Q^2 = 100$  GeV<sup>2</sup>; dash-dotted line:  $Q^2 = 1000$  GeV<sup>2</sup>; full line:  $Q^2 = 10\,000$  GeV<sup>2</sup>.

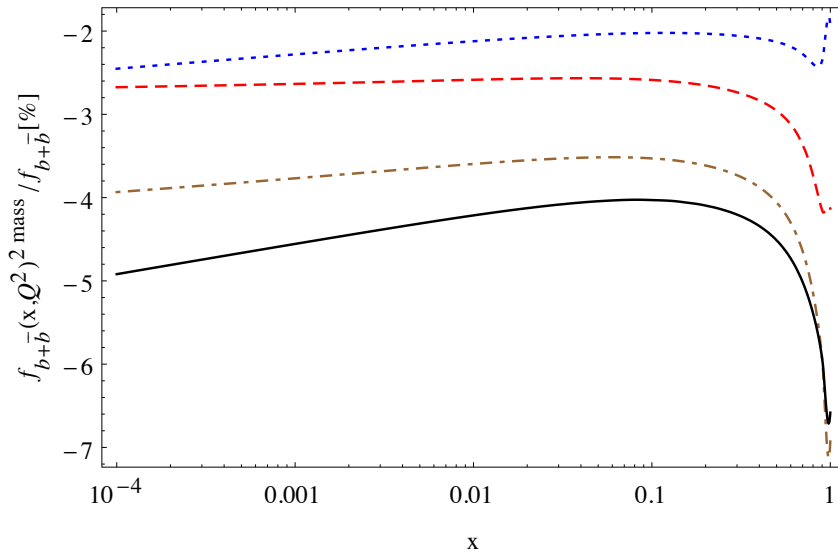


Figure 6.6.: The ratio of the two-mass contribution to the bottom distribution and the complete bottom distribution at  $\mathcal{O}(a_s^2)$ , Equation (6.5) as a function of  $x$  and  $Q^2$  using the parton distribution functions given in Ref. [207] and  $m_c = 1.59 \text{ GeV}$  [208],  $m_b = 4.78 \text{ GeV}$  [357]. Dotted line:  $Q^2 = 50 \text{ GeV}^2$ ; dashed line:  $Q^2 = 100 \text{ GeV}^2$ ; dash-dotted line:  $Q^2 = 1000 \text{ GeV}^2$ ; full line:  $Q^2 = 10\,000 \text{ GeV}^2$ .



# 7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

From 3-loop onwards irreducible diagrams with two massive fermions, phenomenological the charm and bottom quark, contribute to the OMEs. In this chapter the calculation of these contributions to three OMEs, i.e.  $A_{Qq}^{(3),\text{PS}}$ ,  $A_{gg,Q}^{(3)}$  and  $A_{Qg}^{(3)}$ , is presented. The remaining unpolarized OMEs have already been computed in Ref. [202].

In Section 7.1 the calculation of the two mass effects to the pure singlet OME is presented. First the calculational steps and technical details are discussed, then the result in momentum-fraction space will be given. The  $N$ -space solution contains non first-order factorizable contributions and can thus not be expressed in terms of finite nested sums, which are introduced in Appendix C.3, only. However, we present fixed moments not expanded in the ratio  $\eta$  which served as checks for the  $z$ -space results. After this, in Section 7.2, the calculation and result for the gluonic OME  $A_{gg,Q}$  is discussed. In the last section we will present the calculation for the two mass effects to  $A_{Qg}$ . Here the calculational approach is quite different. Since in both spaces non first-order factorizable terms were expected from the start and the complexity of the integrals do not allow for an approach similar to the pure singlet OME the aim was to calculate a large number of moments in an expansion in the ratio  $\eta$ . Therefore we will introduce the technique of the reduction to master integrals and the differential equation approach to Feynman integrals in more detail before turning to the explicit calculation and results for this OME.

## 7.1. The Pure-Singlet Operator Matrix Element $A_{Qq}^{(3),\text{PS}}$

In total there are 16 diagrams contributing to the OME  $\tilde{A}_{Qq}^{(3),\text{PS}}$ . However, using symmetries we can reduce this number to the four diagrams shown in Fig. 7.1. One obtains

$$\tilde{A}_{Qq}^{(3),\text{PS}}(N) = 4(D_{1A}(N) + D_{1B}(N)) + 2(1 + (-1)^N)(D_{2A}(N) + D_{2B}(N)). \quad (7.1)$$

All of the diagrams contain one fermion loop with, cf. Fig. 7.2 ( $b_1$ ) and ( $b_2$ ), and one without operator insertion, cf. Fig. 7.2 ( $a_1$ ). The massive fermion loop without operator insertion can be rendered

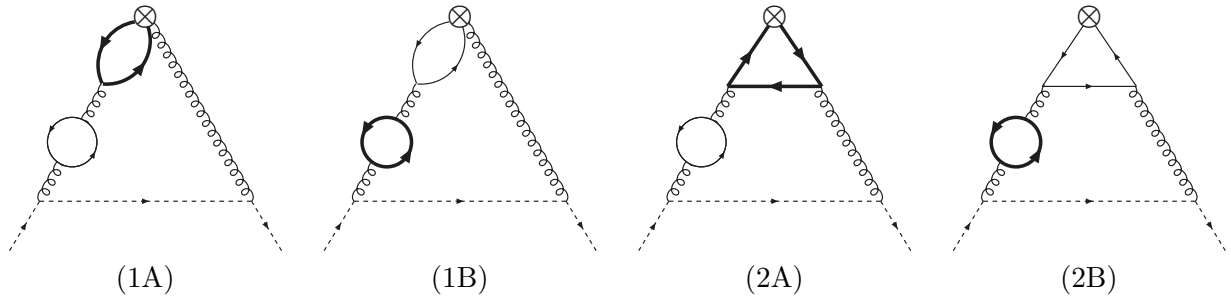


Figure 7.1.: Diagrams contributing to the two mass effects to the pure singlet OME  $A_{Qq}^{\text{PS},(3)}$ . Thick and thin lines represent fermions with different masses.

## 7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

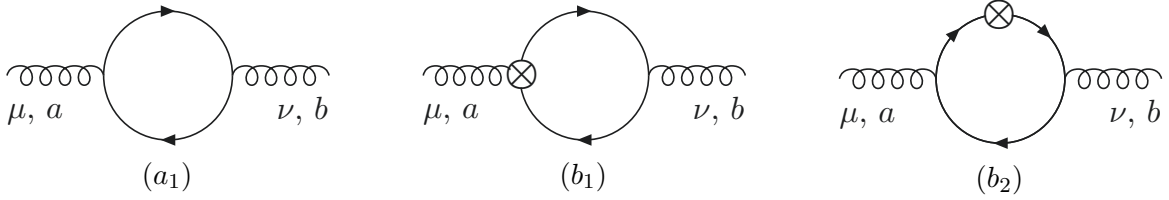


Figure 7.2.: Massive bubble insertions encountered during the calculation of the pure singlet OME. Explicit formulas can be found in Equations (7.2)-(7.4).

effectively massless by using a Mellin-Barnes integral representation, cf. Eq. (C.26),

$$I_{a_1}^{\mu\nu,ab}(k) = 4\delta^{ab}T_F\frac{g_s^2}{\pi}(4\pi)^{-\varepsilon/2}(k_\mu k_\nu - k^2 g_{\mu\nu}) \times \int_{-i\infty}^{+i\infty} d\sigma \left(\frac{m^2}{k^2}\right)^\sigma \frac{\Gamma(\sigma - \varepsilon/2)\Gamma^2(2 - \sigma + \varepsilon/2)\Gamma(-\sigma)}{\Gamma(4 - 2\sigma + \varepsilon)}. \quad (7.2)$$

For the other two bubbles effective Feynman rules derived in Ref. [359] can be used to simplify the expressions. For the operator on the vertex, cf. Fig. 7.2 (b<sub>1</sub>), we have

$$I_{b_1}^{\mu\nu,ab}(k) = 16\delta_{ab}T_F g_s^2 \frac{(\Delta \cdot k)^{N-2}}{(4\pi)^{d/2}} \Gamma(2 - d/2) \int_0^1 dz z^N (1-z) \frac{(\Delta \cdot k)z\Delta_\mu k_\nu - k^2\Delta_\mu\Delta_\nu}{(m^2 - z(1-z)k^2)^{2-d/2}}, \quad (7.3)$$

while the operator on the fermion line, cf. Fig. 7.2 (b<sub>2</sub>), leads to

$$I_{b_2}^{\mu\nu,ab}(k) = 4\delta_{ab}T_F g_s^2 \frac{(\Delta \cdot k)^{N-2}}{(4\pi)^{d/2}} \int_0^1 dz z^{N-2}(1-z) \left[ -2(z(1-z)(g_{\mu\nu}k^2 - 2k_\mu k_\nu) + m^2 g_{\mu\nu}) \frac{z^2\Gamma(3 - d/2)(\Delta \cdot k)^2}{(m^2 - z(1-z)k^2)^{3-d/2}} + \Gamma(2 - d/2)(2Nz + 1 - N) \frac{z(k_\mu\Delta_\nu + k_\nu\Delta_\mu)(\Delta \cdot k)}{(m^2 - z(1-z)k^2)^{2-d/2}} + \Gamma(2 - d/2)((N - 1)(1 - 2z) - dz) \frac{z g_{\mu\nu}(\Delta \cdot k)^2}{(m^2 - z(1-z)k^2)^{2-d/2}} - \Gamma(1 - d/2) \frac{N - 1}{1 - z} (N(1 - z) - 1) \frac{\Delta_\mu\Delta_\nu}{(m^2 - z(1-z)k^2)^{1-d/2}} \right]. \quad (7.4)$$

After inserting these expressions and applying the proper projector, the Dirac algebra which arises in the numerator is performed using FORM [198]. This leads to a linear combination of integrals. The denominators can be combined using Feynman parameters, see Eq. (G.2), and the momentum integrals can then be performed with the help of the relations given in Appendix G. One of the Feynman parameters appears in the form of a Mellin-transform. In order to obtain the result in momentum space this parameter is left unintegrated. For diagram 1A one obtains the expression

$$D_{1A}(N) = -128C_F T_F^2 (1 + (-1)^N) (J_1 - J_2), \quad (7.5)$$

with

$$J_1 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N - 1)}{\Gamma(N + \frac{\varepsilon}{2})} \int_0^1 dz z^{N+\frac{\varepsilon}{2}} (1-z)^{1+\frac{\varepsilon}{2}} B_1\left(\frac{\eta}{z(1-z)}\right), \quad (7.6)$$



$$J_2 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma(N+1+\frac{\varepsilon}{2})} \int_0^1 dz z^{N+\frac{\varepsilon}{2}} (1-z)^{1+\frac{\varepsilon}{2}} B_1\left(\frac{\eta}{z(1-z)}\right). \quad (7.7)$$

$B_1(\xi)$  is the Mellin-Barnes integral left from rendering the fermion loop without operator insertion massless,

$$B_1(\xi) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\sigma \xi^\sigma \Gamma(-\sigma) \Gamma(-\sigma + \varepsilon) \Gamma\left(\sigma - \frac{3\varepsilon}{2}\right) \Gamma\left(\sigma - \frac{\varepsilon}{2}\right) \frac{\Gamma^2(\sigma + 2 - \varepsilon)}{\Gamma(2\sigma + 4 - 2\varepsilon)}. \quad (7.8)$$

The expression for Diagram 2A reads

$$D_{2A}(N) = 64C_F T_F^2 \left\{ -\frac{1}{4}(\varepsilon + 2) [-2J_3 + 2\eta J_4 + (2N + 2 + \varepsilon)J_5 - (N - 1)J_6] + N(N - 1)(J_7 - J_8) - (N - 1)(J_9 - J_{10}) \right\}, \quad (7.9)$$

with

$$J_3 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma(N+2+\frac{\varepsilon}{2})} \int_0^1 dz z^{N+\frac{\varepsilon}{2}} (1-z)^{1+\frac{\varepsilon}{2}} B_2\left(\frac{\eta}{z(1-z)}\right), \quad (7.10)$$

$$J_4 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma(N+2+\frac{\varepsilon}{2})} \int_0^1 dz z^{N-1+\frac{\varepsilon}{2}} (1-z)^{\frac{\varepsilon}{2}} B_3\left(\frac{\eta}{z(1-z)}\right), \quad (7.11)$$

$$J_5 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma(N+2+\frac{\varepsilon}{2})} \int_0^1 dz z^{N+\frac{\varepsilon}{2}} (1-z)^{1+\frac{\varepsilon}{2}} B_1\left(\frac{\eta}{z(1-z)}\right), \quad (7.12)$$

$$J_6 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma(N+2+\frac{\varepsilon}{2})} \int_0^1 dz z^{N-1+\frac{\varepsilon}{2}} (1-z)^{1+\frac{\varepsilon}{2}} B_1\left(\frac{\eta}{z(1-z)}\right), \quad (7.13)$$

$$J_7 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N-1)}{\Gamma(N+\frac{\varepsilon}{2})} \int_0^1 dz z^{N-1+\frac{\varepsilon}{2}} (1-z)^{2+\frac{\varepsilon}{2}} B_4\left(\frac{\eta}{z(1-z)}\right), \quad (7.14)$$

$$J_8 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma(N+1+\frac{\varepsilon}{2})} \int_0^1 dz z^{N-1+\frac{\varepsilon}{2}} (1-z)^{2+\frac{\varepsilon}{2}} B_4\left(\frac{\eta}{z(1-z)}\right), \quad (7.15)$$

$$J_9 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N-1)}{\Gamma(N+\frac{\varepsilon}{2})} \int_0^1 dz z^{N-1+\frac{\varepsilon}{2}} (1-z)^{1+\frac{\varepsilon}{2}} B_4\left(\frac{\eta}{z(1-z)}\right), \quad (7.16)$$

$$J_{10} = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma(N+1+\frac{\varepsilon}{2})} \int_0^1 dz z^{N-1+\frac{\varepsilon}{2}} (1-z)^{1+\frac{\varepsilon}{2}} B_4\left(\frac{\eta}{z(1-z)}\right). \quad (7.17)$$

The Mellin-Barnes integrals needed to express  $D_{2A}(N)$  are

$$B_2(\xi) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\sigma \xi^\sigma \Gamma(-\sigma) \Gamma(-\sigma + \varepsilon) \Gamma\left(\sigma - \frac{3\varepsilon}{2}\right) \Gamma\left(\sigma + 1 - \frac{\varepsilon}{2}\right) \frac{\Gamma^2(\sigma + 2 - \varepsilon)}{\Gamma(2\sigma + 4 - 2\varepsilon)}, \quad (7.18)$$

$$B_3(\xi) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\sigma \xi^\sigma \Gamma(-\sigma) \Gamma(-\sigma - 1 + \varepsilon) \Gamma\left(\sigma + 1 - \frac{3\varepsilon}{2}\right) \Gamma\left(\sigma + 1 - \frac{\varepsilon}{2}\right) \times \frac{\Gamma^2(\sigma + 3 - \varepsilon)}{\Gamma(2\sigma + 6 - 2\varepsilon)}, \quad (7.19)$$

$$B_4(\xi) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\sigma \xi^\sigma \Gamma(-\sigma) \Gamma(-\sigma + \varepsilon) \Gamma\left(\sigma - \frac{3\varepsilon}{2}\right) \Gamma\left(\sigma - 1 - \frac{\varepsilon}{2}\right) \frac{\Gamma^2(\sigma + 2 - \varepsilon)}{\Gamma(2\sigma + 4 - 2\varepsilon)}.$$

The expression for the other mass assignment, i.e. diagrams 1B and 2B, can be obtained by setting  $\eta \rightarrow 1/\eta$ .

### 7.1.1. The $N$ -space solution

The calculation of the  $N$ -space solution for  $A_{Qq}^{(3),\text{PS}}$  seems to be straight forward. We can integrate the last remaining Feynman parameter in terms of Beta-functions and are left with a Mellin-Barnes integral over a rational expression of  $\Gamma$ -functions. This integral can be solved by closing the integration contour to the converging side and sum up residues. This procedure can be further simplified by using the packages MB [360] and MBresolve [361]. In this way poles in the dimensional regulator  $\varepsilon$  can be extracted by taking appropriate residues beforehand and an integration contour is found so the remaining integral is finite. We are only left with single infinite sums to calculate  $A_{Qq}^{(3),\text{PS}}$ .

For example for  $J_1^B$  we find

$$\begin{aligned}
J_1^B = & \left( \frac{m_2^2}{\mu^2} \right)^{\frac{3}{2}\varepsilon} \left\{ \frac{1}{\varepsilon^3} \left\{ \frac{8}{9(N-1)(N+1)(N+2)} \right\} + \frac{1}{\varepsilon^2} \left\{ \frac{4(6+20N+12N^2+N^3)}{27(N-1)N(N+1)^2(N+2)^2} \right. \right. \\
& - \frac{2}{3(N-1)(N+1)(N+2)} \ln(\eta) - \frac{2}{9(N-1)(N+1)(N+2)} S_1 \left. \right\} \\
& + \frac{1}{\varepsilon} \left\{ -\frac{2+7N+2N^2-N^3}{3(N-1)N(N+1)^2(N+2)^2} \ln(\eta) + \frac{1}{3(N-1)(N+1)(N+2)} \ln^2(\eta) \right. \\
& + \frac{132+698N+882N^2+617N^3+300N^4+71N^5}{81(N-1)N(N+1)^3(N+2)^3} - \frac{6+17N+30N^2+13N^3}{27(N-1)N(N+1)^2(N+2)^2} S_1 \\
& + \frac{1}{9(N-1)(N+1)(N+2)} S_1^2 + \frac{4}{9(N-1)(N+1)(N+2)} S_2 + \frac{1}{3(N-1)(N+1)(N+2)} \zeta_2 \left. \right\} \\
& - \frac{5}{36(N-1)(N+1)(N+2)} \ln^3(\eta) - \frac{(-6-22N+7N^3)}{18(N-1)N(N+1)^2(N+2)^2} \ln^2(\eta) \\
& + \frac{2352+14068N+21720N^2+19671N^3+14259N^4+7005N^5+1629N^6+80N^7}{486(N-1)N(N+1)^4(N+2)^4} \\
& - \left[ \frac{72+406N+351N^2+163N^3+117N^4+43N^5}{54(N-1)N(N+1)^3(N+2)^3} + \frac{1}{4(N-1)(N+1)(N+2)} \zeta_2 \right] \ln(\eta) \\
& + \left[ \frac{1}{12(N-1)(N+1)(N+2)} \ln^2(\eta) - \frac{1-6N-4N^2}{9(N-1)(N+1)^2(N+2)^2} \ln(\eta) \right. \\
& - \frac{48+178N+711N^2+745N^3+249N^4+13N^5}{162(N-1)N(N+1)^3(N+2)^3} + \frac{5}{36(N-1)(N+1)(N+2)} S_2 \\
& - \frac{1}{12(N-1)(N+1)(N+2)} \zeta_2 \left. \right] S_1 + \left[ \frac{6+20N+12N^2+N^3}{54(N-1)N(N+1)^2(N+2)^2} \right. \\
& - \frac{1}{12(N-1)(N+1)(N+2)} \ln(\eta) \left. \right] S_1^2 - \frac{1}{108(N-1)(N+1)(N+2)} S_1^3 \\
& + \left[ \frac{24+89N-6N^2-32N^3}{54(N-1)N(N+1)^2(N+2)^2} - \frac{7}{12(N-1)(N+1)(N+2)} \ln(\eta) \right] S_2 \\
& + \frac{13}{27(N-1)(N+1)(N+2)} S_3 + \frac{6+20N+12N^2+N^3}{18(N-1)N(N+1)^2(N+2)^2} \zeta_2 \\
& - \frac{1}{9(N-1)(N+1)(N+2)} \zeta_3
\end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{2\pi i} \frac{1}{N-1} \int_{-0.2-i\infty}^{-0.2+i\infty} d\sigma \eta^{-\sigma} \frac{\Gamma(2-\sigma)\Gamma(2+\sigma)\Gamma(N+1-\sigma)\Gamma^2(\sigma)\Gamma^2(-\sigma)}{\Gamma(4+2\sigma)\Gamma(N+3-2\sigma)} \\
 & + \mathcal{O}(\varepsilon), \left. \vphantom{\int} \right\} \tag{7.21}
 \end{aligned}$$

where the last integral can be converted into an infinite sum by closing the integration to left. After taking residues at  $\sigma = -1$  and  $\sigma = -2$  it is straight forward to obtain a closed form solution for the residues at  $\sigma = -3, -4, \dots$  containing harmonic sums at arguments involving the expressions  $k + N$  and  $k + N/2$ . Even for this single integral the expression obtained is lengthy and will not be given here. The poles are obtained analytically in  $N$  and have been checked against the terms expected from renormalization. This procedure can be applied to all contributing integrals to obtain a closed form solution for  $A_{Qq}^{(3),PS}$  in terms of infinite sums.

However, the resulting difference equations for these last sums turn out to be not first-order factorizable. This means that the symbolic summation package `Sigma` [268, 269] cannot find closed form solutions for these sums in terms of indefinitely nested product sum expressions introduced in Appendix C.3. Nevertheless for fixed integer  $N$  the problem simplifies and the resulting sums are solvable in a closed form. The corresponding expressions up to  $N = 10$  can be found in Appendix I. Moments up to  $N = 200$  have been calculated, however, since the expressions get longer and longer with rising  $N$  we do not give them here. Although the fixed moments formally depend on the square root of  $\eta$  the expansion therein shows that the OME only depends on  $\eta$  itself. This behaviour is expected since Eq. (7.21) effectively defines a Taylor expansion around  $\eta = 0$ . These fixed moments were used to cross-check the result in momentum space, which will be presented in the following.

### 7.1.2. The Momentum-space Solution

For the momentum space solution we want to leave the last Feynman parameter unintegrated and compute the remainder as Laurent series in  $\varepsilon$ . Therefore the integrals  $B_i$  have to be solved as an expansion in  $\varepsilon$ . To do this we can again facilitate the packages `MB` [360] and `MBresolve` [361] to extract the poles of the Laurent series and are left with single Mellin-Barnes integrals which have to be solved to obtain the full  $\mathcal{O}(\varepsilon^0)$  part. We split the contour integrals

$$B_i(\xi) = B_i^{(\varepsilon)}(\xi) + B_i^{(0)}(\xi), \quad i = 1, 2, 3, 4, \tag{7.22}$$

where  $B_i^{(\varepsilon)}(\xi)$  are the residues containing the poles while  $B_i^{(0)}(\xi)$  is the remaining finite contour integral. The  $B_i^{(0)}(\xi)$  are given by

$$B_1^{(0)}(\xi) = \frac{1}{2\pi i} \int_{-1/2-i\infty}^{-1/2+i\infty} d\sigma \xi^\sigma \Gamma^2(-\sigma)\Gamma^2(\sigma) \frac{\Gamma^2(\sigma+2)}{\Gamma(2\sigma+4)} + \mathcal{O}(\varepsilon), \tag{7.23}$$

$$B_2^{(0)}(\xi) = \frac{1}{2\pi i} \int_{-1/2-i\infty}^{-1/2+i\infty} d\sigma \xi^\sigma \Gamma^2(-\sigma)\Gamma(\sigma)\Gamma(\sigma+1) \frac{\Gamma^2(\sigma+2)}{\Gamma(2\sigma+4)} + \mathcal{O}(\varepsilon), \tag{7.24}$$

$$B_3^{(0)}(\xi) = \frac{1}{2\pi i} \int_{-1/2-i\infty}^{-1/2+i\infty} d\sigma \xi^\sigma \Gamma(-\sigma)\Gamma(-\sigma-1)\Gamma^2(\sigma+1) \frac{\Gamma^2(\sigma+3)}{\Gamma(2\sigma+6)} + \mathcal{O}(\varepsilon), \tag{7.25}$$

$$B_4^{(0)}(\xi) = \frac{1}{2\pi i} \int_{-1/2-i\infty}^{-1/2+i\infty} d\sigma \xi^\sigma \Gamma^2(-\sigma)\Gamma(\sigma)\Gamma(\sigma-1) \frac{\Gamma^2(\sigma+2)}{\Gamma(2\sigma+4)} + \mathcal{O}(\varepsilon). \tag{7.26}$$

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Note that  $N$ -dependent pre-factors have been stripped off from the  $B_i$  and that Eq. 7.9 also contains these kind of factors. Some of the integrals will therefore be left with a factor of the form

$$\frac{1}{N+l}, \quad \text{with } l \in \{-1, 0, 1\}. \quad (7.27)$$

In order to arrive at a genuine Mellin transform, these factors need to be absorbed into the integrals. This can be achieved by using the following integration by parts identities

$$\frac{1}{N+l} \int_a^b dz z^{N-1} f(z) = \frac{b^{N+l}}{N+l} \int_a^b dy \frac{f(y)}{y^{l+1}} - \int_a^b dz z^{N+l-1} \int_a^z dy \frac{f(y)}{y^{l+1}} \quad (7.28)$$

$$= \frac{a^{N+l}}{N+l} \int_a^b dy \frac{f(y)}{y^{l+1}} + \int_a^b dz z^{N+l-1} \int_z^b dy \frac{f(y)}{y^{l+1}}. \quad (7.29)$$

For more general  $N$ -dependent pre-factors one can use convolution identities to arrive at one-dimensional integral representations. More details on these will be presented in Section 7.2 where this problem is encountered. Therefore the result for  $A_{Qq}^{(3),\text{PS}}$  will contain a single integration which has to be performed numerically.

To solve the integrals (7.23) to (7.26) we have to close the contour to the converging side. Applying Legendre's duplication formula

$$\Gamma(2\sigma + 2l) = \frac{4^{\sigma+l}}{2\sqrt{\pi}} \Gamma(\sigma + l) \Gamma\left(\sigma + l + \frac{1}{2}\right), \quad l = 2, 3, \quad (7.30)$$

to the  $\Gamma$ -functions in the denominator we see that we have to demand  $\xi < 4$  to arrive at a convergent integral for the closure to the right and  $\xi > 4$  for the closure to the left. Since for diagrams 1B and 2B

$$\xi = \frac{1}{\eta z(1-z)} > 4, \quad \text{for } z \in (0, 1) \quad (7.31)$$

we can simply close the contour to the left and sum up the residues. For diagrams 1A and 2A

$$\xi = \frac{\eta}{z(1-z)} < 4, \quad \text{for } z \in (\eta_-, \eta_+), \quad (7.32)$$

$$\xi = \frac{\eta}{z(1-z)} > 4, \quad \text{for } z \in (0, \eta_-) \quad \text{and} \quad z \in (\eta_+, 1), \quad (7.33)$$

with

$$\eta_{\pm} = \frac{1}{2} \left( 1 \pm \sqrt{1-\eta} \right). \quad (7.34)$$

For diagrams 1A and 2A we therefore have to close to the right for  $0 < z < \eta_-$  and  $\eta_+ < z < 1$  and to the left if  $\eta_- < z < \eta_+$ . This will lead to functions with restricted support in  $z$  in the final result.

Closing the contour to the right and summing residues, we obtain

$$B_1^{(0)}(\xi) = -\left(\frac{\zeta_2}{6} + \frac{14}{27}\right) \ln(\xi) - \frac{1}{36} \ln^3(\xi) + \frac{5}{36} \ln^2(\xi) + \frac{5}{18} \zeta_2 - \frac{\zeta_3}{3} + \frac{82}{81} + \sum_{k=1}^{\infty} \xi^k \frac{\Gamma^2(k+2)}{k^2 \Gamma(2k+4)} \left( 2S_1(2k+3) - 2S_1(k) + \frac{2}{k(k+1)} - \ln(\xi) \right), \quad (7.35)$$

$$B_2^{(0)}(\xi) = -\frac{1}{12} \ln^2(\xi) + \frac{5}{18} \ln(\xi) - \frac{\zeta_2}{6} - \frac{14}{27} + \sum_{k=1}^{\infty} \xi^k \frac{\Gamma^2(k+2)}{k \Gamma(2k+4)} \left( 2S_1(2k+3) - 2S_1(k) - \frac{k-1}{k(k+1)} - \ln(\xi) \right), \quad (7.36)$$

$$B_3^{(0)}(\xi) = \sum_{k=0}^{\infty} \xi^k \frac{\Gamma^2(k+3)}{(k+1)\Gamma(2k+6)} \left( 2S_1(k+2) - 2S_1(2k+5) - \frac{1}{k+1} + \ln(\xi) \right), \quad (7.37)$$

$$\begin{aligned} B_4^{(0)}(\xi) &= -\left(\frac{\xi}{30} + \frac{1}{9}\right) \zeta_2 + \left(\frac{107\xi}{900} + \frac{\zeta_2}{6} + \frac{11}{27}\right) \ln(\xi) - \frac{4067}{13500}\xi + \frac{1}{36} \ln^3(\xi) \\ &\quad - \left(\frac{\xi}{60} + \frac{1}{18}\right) \ln^2(\xi) + \frac{\zeta_3}{3} - \frac{49}{81} + \sum_{k=2}^{\infty} \xi^k \frac{\Gamma^2(k+2)}{(k-1)k^2\Gamma(2k+4)} \left( 2S_1(2k+3) \right. \\ &\quad \left. - 2S_1(k) + \frac{k^2+3k-2}{(k-1)k(k+1)} - \ln(\xi) \right), \end{aligned} \quad (7.38)$$

while closing to the left leads to

$$\begin{aligned} B_1^{(0)}(\xi) &= \frac{1}{\xi} \ln(\xi) + \sum_{k=2}^{\infty} \xi^{-k} \frac{\Gamma(2k-3)}{k^2\Gamma^2(k-1)} \left[ \ln(\xi) \left( 4S_1(k) - 4S_1(2k-4) - \frac{4}{k-1} \right) \right. \\ &\quad \left. + \ln^2(\xi) + 4S_1^2(k) + 4S_1^2(2k-4) - 8S_1(k) \left( S_1(2k-4) + \frac{1}{k-1} \right) \right. \\ &\quad \left. + \frac{8}{k-1} S_1(2k-4) + 2S_2(k) - 4S_2(2k-4) + \frac{2}{(k-1)^2} + 2\zeta_2 \right], \end{aligned} \quad (7.39)$$

$$\begin{aligned} B_2^{(0)}(\xi) &= \frac{1}{\xi} - \frac{\ln(\xi)}{\xi} + \sum_{k=2}^{\infty} \xi^{-k} \frac{\Gamma(2k-3)}{k\Gamma^2(k-1)} \left[ \ln(\xi) \left( 4S_1(2k-4) - 4S_1(k) + \frac{2(3k-1)}{(k-1)k} \right) \right. \\ &\quad \left. - \ln^2(\xi) - 2S_2(k) - 4S_1^2(k) - 4S_1^2(2k-4) + 4S_2(2k-4) - \frac{2(3k-2)}{(k-1)^2k} \right. \\ &\quad \left. - \frac{4(3k-1)}{(k-1)k} S_1(2k-4) + 4S_1(k) \left( 2S_1(2k-4) + \frac{3k-1}{(k-1)k} \right) - 2\zeta_2 \right], \end{aligned} \quad (7.40)$$

$$\begin{aligned} B_3^{(0)}(\xi) &= -\frac{14}{27\xi} - \frac{\zeta_2}{6\xi} + \frac{5}{18\xi} \ln(\xi) - \frac{1}{12\xi} \ln^2(\xi) - \frac{1}{\xi^2} + \frac{1}{\xi^2} \ln(\xi) \\ &\quad + \sum_{k=3}^{\infty} \xi^{-k} \frac{(k-2)\Gamma(2k-5)}{\Gamma(k-2)\Gamma(k)} \left[ \ln(\xi) \left( 4S_1(k-3) - 4S_1(2k-6) + \frac{2}{k-1} \right) \right. \\ &\quad \left. + 4S_1^2(k-3) + 4S_1^2(2k-6) + 4S_1(k-3) \left( \frac{1}{k-1} - 2S_1(2k-6) \right) + 2\zeta_2 \right. \\ &\quad \left. - \frac{4}{k-1} S_1(2k-6) + 2S_2(k-3) - 4S_2(2k-6) + \frac{2}{(k-1)^2} + \ln^2(\xi) \right], \end{aligned} \quad (7.41)$$

$$\begin{aligned} B_4^{(0)}(\xi) &= -\frac{1}{4\xi} - \frac{\ln(\xi)}{2\xi} + \sum_{k=2}^{\infty} \xi^{-k} \frac{(k-1)\Gamma(2k-3)}{k\Gamma(k-1)\Gamma(k+2)} \left[ 4S_2(2k-4) - S_2(k+1) \right. \\ &\quad \left. - \ln^2(\xi) + \ln(\xi) \left( 4S_1(2k-4) - 2S_1(k) - 2S_1(k+1) + \frac{4}{k-1} \right) \right. \\ &\quad \left. - 4S_1^2(2k-4) - \frac{8}{k-1} S_1(2k-4) + 4S_1(k+1) \left( S_1(2k-4) + \frac{1}{k-1} \right) \right. \\ &\quad \left. + S_1(k) \left( 4S_1(2k-4) - 2S_1(k+1) + \frac{4}{k-1} \right) - S_1^2(k) - S_1^2(k+1) \right. \\ &\quad \left. - S_2(k) - \frac{2}{(k-1)^2} - 2\zeta_2 \right]. \end{aligned} \quad (7.42)$$

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In the above expressions ratios of  $\Gamma$ -functions are related to special binomial coefficients, like

$$\frac{\Gamma^2(k+1)}{\Gamma(2k+2)} = \frac{1}{2k} \frac{1}{\binom{2k}{k}}. \quad (7.43)$$

All of the above sums can be performed using the packages `Sigma` [268, 269], `HarmonicSums` [240, 273, 275] and `EvaluateMultiSums` [271]. The results are expressed in terms of generalized iterated integrals, cf. Appendix C.4.

We obtain the following expression for the  $\mathcal{O}(\varepsilon^0)$  term of the unrenormalized 3-loop two-mass pure singlet operator matrix element

$$\begin{aligned} \tilde{a}_{Qq}^{(3),\text{PS}}(z) = & C_F T_F^2 \left\{ R_0(m_1, m_2, z) + (\theta(\eta_- - z) + \theta(z - \eta_+)) z g_0(\eta, z) \right. \\ & + \theta(\eta_+ - z) \theta(z - \eta_-) \left[ z f_0(\eta, z) \right. \\ & \left. - \int_{\eta_-}^z dy \left( f_1(\eta, y) + \frac{y}{z} f_2(\eta, y) + \frac{z}{y} f_3(\eta, y) \right) \right] \\ & + \theta(\eta_- - z) \int_z^{\eta_-} dy \left( g_1(\eta, y) + \frac{y}{z} g_2(\eta, y) + \frac{z}{y} g_3(\eta, y) \right) \\ & - \theta(z - \eta_+) \int_{\eta_+}^z dy \left( g_1(\eta, y) + \frac{y}{z} g_2(\eta, y) + \frac{z}{y} g_3(\eta, y) \right) \\ & + z h_0(\eta, z) + \int_z^1 dy \left( h_1(\eta, y) + \frac{y}{z} h_2(\eta, y) + \frac{z}{y} h_3(\eta, y) \right) \\ & + \theta(\eta_+ - z) \int_{\eta_-}^{\eta_+} dy \left( f_1(\eta, y) + \frac{y}{z} f_2(\eta, y) + \frac{z}{y} f_3(\eta, y) \right) \\ & \left. + \int_{\eta_+}^1 dy \left( g_1(\eta, y) + \frac{y}{z} g_2(\eta, y) + \frac{z}{y} g_3(\eta, y) \right) \right\}. \quad (7.44) \end{aligned}$$

Here  $\theta(z)$  denotes the Heaviside function

$$\theta(z) = \begin{cases} 1 & z \geq 0 \\ 0 & z < 0. \end{cases} \quad (7.45)$$

The function  $R_0(m_1, m_2, z)$  arises from the residues taken in order to resolve the singularities in  $\varepsilon$  of the contour integrals, see Eq. (7.22). The functions  $f_i(\eta, z)$ ,  $g_i(\eta, z)$  and  $h_i(\eta, z)$ , with  $i = 0, 1, 2, 3$ , arise from the sum of residues of the contour integrals that remain after the  $\varepsilon$  expansion, as described in the previous section. The functions with  $i = 0$  are those where no additional factor depending on  $N$  needed to be absorbed. The functions with  $i = 1$ ,  $i = 2$  and  $i = 3$  are those where a factor of  $1/N$ ,  $1/(N-1)$  and  $1/(N+1)$  was absorbed, respectively, see Eqs. (7.28, 7.29). The different Heaviside  $\theta$  functions restrict the corresponding values of  $z$  to the appropriate regions.

Since no contour integral needs to be performed in the case of  $R_0(m_1, m_2, z)$ , the easiest way to compute this function is to integrate in  $z$  and then perform the Mellin inversion using `HarmonicSums`. We obtain,

$$\begin{aligned} R_0(m_1, m_2, z) = & 32 (L_1^3 + L_1^2 L_2 + L_1 L_2^2 + L_2^3) \left[ \frac{P_0}{3z} - 2(z+1) H_0 \right] \\ & + 32 (L_1^2 + L_2^2) \left[ 2(z+1) \left( H_{0,0} + \frac{1}{3} H_{0,1} - \frac{\zeta_2}{3} \right) - \frac{P_0 H_1}{9z} \right] \end{aligned}$$

$$\begin{aligned}
 & -\frac{1}{9}(4z+5)(7z+5)H_0 + \frac{z-1}{27z}(170z^2+53z+80) \Big] \\
 & +128L_1L_2 \left[ \frac{z-1}{27z}(56z^2+47z+20) + \frac{2}{3}(z+1)(H_{0,1}-\zeta_2) \right. \\
 & \left. -\frac{4}{9}(z^2+7z+4)H_0 - \frac{P_0H_1}{9z} \right] + \frac{128\zeta_3}{27z}(64z^3+35z^2-25z+8) \\
 & +64(L_1+L_2) \left[ (z+1) \left( \frac{29}{9}H_{0,1} - \frac{4}{3}H_{0,0,0} + \frac{2}{3}H_{0,0,1} + 2H_{0,1,0} \right. \right. \\
 & \left. \left. -\frac{4}{3}H_{0,1,1} - \frac{8}{3}\zeta_2H_0 + \frac{14}{3}\zeta_3 \right) + \frac{z-1}{27z}(260z^2+231z+116) \right. \\
 & \left. +\frac{P_0}{3z} \left( \frac{2}{3}H_{1,1} - H_{1,0} \right) + \frac{2\zeta_2}{9z}(6z^3-10z^2-19z-6) \right. \\
 & \left. -\frac{1}{27}(168z^2+265z+229)H_0 - \frac{4(z-1)}{27z}(5z^2+23z+5)H_1 \right. \\
 & \left. +\frac{2}{9}(6z^2+4z-5)H_{0,0} \right] + \frac{64\zeta_2}{81z}(282z^3-229z^2-85z-120) \\
 & +\frac{64P_0}{9z} \left( 4H_{1,0,0} - 2H_{1,0,1} - 2H_{1,1,0} - \frac{2}{3}H_{1,1,1} + \zeta_2H_1 \right) \\
 & +128(z+1) \left( \frac{2}{9}(6z-5)H_{0,1,0} + \frac{8}{9}H_{0,0,0,0} - \frac{4}{9}H_{0,0,0,1} - \frac{4}{3}H_{0,0,1,0} \right. \\
 & \left. +\frac{2}{9}H_{0,0,1,1} - \frac{4}{3}H_{0,1,0,0} + \frac{2}{3}H_{0,1,0,1} - 2\zeta_3H_0 + \frac{2}{3}H_{0,1,1,0} + \frac{2}{9}H_{0,1,1,1} \right. \\
 & \left. +\frac{7}{9}\zeta_2H_{0,0} - \frac{1}{3}\zeta_2H_{0,1} + \frac{8}{15}\zeta_2^2 \right) - \frac{128}{27}(12z^2+19z+19)H_{0,1,1} \\
 & -\left( \frac{256}{243}(813z^2+29z+263) + \frac{64}{27}\zeta_2(60z^2+91z+37) \right) H_0 \\
 & +\frac{128(z-1)}{81z}(22z^2-25z+4)H_1 + \frac{256}{81}(84z^2+109z+100)H_{0,0} \\
 & +\frac{256}{27}(6z^2-5z-5)H_{0,0,1} - \frac{128(z-1)}{27z}(56z^2-43z+20)H_{1,0} \\
 & +\frac{128(z-1)}{81z}(40z^2+49z+40)H_{1,1} - \frac{256}{27}(12z^2-z-10)H_{0,0,0} \\
 & +\frac{128}{81}(47z+29)H_{0,1} + \frac{256(z-1)}{729z}(2602z^2-203z+1360), \tag{7.46}
 \end{aligned}$$

where

$$P_0 = (z-1)(4+7z+4z^2), \tag{7.47}$$

$L_1$  and  $L_2$  are the logarithms defined in Eq. (5.3), and we used the shorthand notation  $H_{\vec{a}}(z) \equiv H_{\vec{a}}$ . In principle (7.46) could still be reduced to a shorter basis using shuffle-algebra [286].

The  $f_i(\eta, z)$  functions, which are defined in the range  $\eta_- < z < \eta_+$ , are given by

$$\begin{aligned}
 f_0(\eta, z) &= \frac{8P_{88}(4z(1-z)-\eta)^{3/2}}{45\eta^{3/2}(z-1)z^3} K_1 \left( \frac{\eta}{z(1-z)} \right) - \frac{16(z-1)}{3z} \left\{ K_2 \left( \frac{\eta}{z(1-z)} \right) \right. \\
 & \left. - \frac{2(6\eta+30z^2-5z)}{15z} \left[ 2\zeta_2 + \ln^2 \left( \frac{\eta}{z(1-z)} \right) \right] \right\} + \frac{P_{86}}{90(z-1)^3z^5}
 \end{aligned}$$

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$$+\frac{2P_{87}}{45(z-1)^3z^5}\ln\left(\frac{\eta}{z(1-z)}\right), \quad (7.48)$$

$$\begin{aligned} f_1(\eta, z) = & -\frac{16P_{91}(4z(1-z)-\eta)^{3/2}}{45\eta^{3/2}(z-1)z^3}K_1\left(\frac{\eta}{z(1-z)}\right)+\frac{4P_{90}}{45(z-1)^3z^5}\ln\left(\frac{\eta}{z(1-z)}\right) \\ & +\frac{32(z-1)(4z+1)}{3z}K_2\left(\frac{\eta}{z(1-z)}\right)-\frac{64P_{92}}{45z^2}\left[2\zeta_2+\ln^2\left(\frac{\eta}{z(1-z)}\right)\right] \\ & -\frac{P_{89}}{45(z-1)^3z^5}, \end{aligned} \quad (7.49)$$

$$\begin{aligned} f_2(\eta, z) = & \frac{64P_{95}(4z(1-z)-\eta)^{3/2}}{9\eta^{3/2}(z-1)z^2}K_1\left(\frac{\eta}{z(1-z)}\right)-\frac{128}{3}(z-1)\left[K_2\left(\frac{\eta}{z(1-z)}\right)\right. \\ & \left.-\frac{10}{3}\ln^2\left(\frac{\eta}{z(1-z)}\right)-\frac{20}{3}\zeta_2\right]-\frac{4}{9(z-1)^3z^4}\left[4P_{94}\ln\left(\frac{\eta}{z(1-z)}\right)-P_{93}\right], \end{aligned} \quad (7.50)$$

$$\begin{aligned} f_3(\eta, z) = & -\frac{16P_{98}\sqrt{4z(1-z)-\eta}}{9\eta^{3/2}(z-1)z^3}K_1\left(\frac{\eta}{z(1-z)}\right)-\frac{32(z-1)}{3z}\left\{K_2\left(\frac{\eta}{z(1-z)}\right)\right. \\ & \left.-\frac{2}{3}(3z+5)\left[2\zeta_2+\ln^2\left(\frac{\eta}{z(1-z)}\right)\right]\right\}+\frac{4P_{97}}{9(z-1)^3z^5}\ln\left(\frac{\eta}{z(1-z)}\right) \\ & -\frac{P_{96}}{27(z-1)^3z^5}, \end{aligned} \quad (7.51)$$

where the functions  $K_1$  and  $K_2$ , which appear repeatedly in the expressions above, are given by

$$K_1(u) = G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, u\right) + \frac{1}{2}(1-2\ln(u))G\left(\{\sqrt{4-\tau}\sqrt{\tau}\}, u\right), \quad (7.52)$$

$$\begin{aligned} K_2(u) = & -G\left(\{\sqrt{4-\tau}\sqrt{\tau}\}, u\right)G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, u\right) + \frac{2}{3}\ln^3(u) \\ & + G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, u\right) + 4\zeta_2\ln(u) + 8\zeta_3 \\ & - \frac{1}{4}(1-2\ln(u))G^2\left(\{\sqrt{4-\tau}\sqrt{\tau}\}, u\right). \end{aligned} \quad (7.53)$$

The expressions of the  $G$ -functions are presented in Appendix H.1 in terms of harmonic polylogarithms containing square-root valued arguments, and the  $P_i$ 's, with  $i = 1, \dots, 13$ , are polynomials in  $\eta$  and  $z$  given by

$$\begin{aligned} P_{86} = & 1536(z-1)^4(3z+2)z^4 + 576(z-1)^3(12z-7)\eta z^3 \\ & + 8(z-1)^2(264z-329)\eta^2 z^2 + 16(z-1)(12z-37)\eta^3 z - 45\eta^4, \end{aligned} \quad (7.54)$$

$$\begin{aligned} P_{87} = & 128(z-1)^4(3z-8)z^4 - 32(z-1)^3(33z-8)\eta z^3 \\ & - 4(z-1)^2(108z-133)\eta^2 z^2 - 24(z-1)(2z-7)\eta^3 z + 15\eta^4, \end{aligned} \quad (7.55)$$

$$P_{88} = 4(z-1)^2(6z-1)z^2 - 6(z-1)(4z+1)\eta z + 15\eta^2, \quad (7.56)$$

$$\begin{aligned} P_{89} = & 768(z-1)^4(40z+7)z^4 + 576(z-1)^3(20z-1)\eta z^3 \\ & - 8(z-1)^2(260z+197)\eta^2 z^2 - 16(z-1)(100z+31)\eta^3 z - 45(4z+1)\eta^4, \end{aligned} \quad (7.57)$$

$$\begin{aligned} P_{90} = & 64(z-1)^4(40z+13)z^4 + 16(z-1)^3(200z+17)\eta z^3 \\ & - 4(z-1)^2(100z+79)\eta^2 z^2 - 48(z-1)(10z+3)\eta^3 z - 15(4z+1)\eta^4, \end{aligned} \quad (7.58)$$

$$P_{91} = 8(z-1)^2(10z+1)z^2 - 6(z-1)(20z+3)\eta z + 15(4z+1)\eta^2, \quad (7.59)$$

$$P_{92} = 10(z-1)z(10z+1) - 3\eta, \quad (7.60)$$



$$P_{93} = 1536(z-1)^4 z^4 + 576(z-1)^3 \eta z^3 - 104(z-1)^2 \eta^2 z^2 - 80(z-1) \eta^3 z - 9\eta^4, \quad (7.61)$$

$$P_{94} = 128(z-1)^4 z^4 + 160(z-1)^3 \eta z^3 - 20(z-1)^2 \eta^2 z^2 - 24(z-1) \eta^3 z - 3\eta^4, \quad (7.62)$$

$$P_{95} = 4(z-1)^2 z^2 - 6(z-1) \eta z + 3\eta^2, \quad (7.63)$$

$$P_{96} = 512(z-1)^4 (7z-9) z^4 - 1728(z-1)^3 (2z+1) \eta z^3 - 24(z-1)^2 (24z-13) \eta^2 z^2 + 240(z-1) \eta^3 z + 27\eta^4, \quad (7.64)$$

$$P_{97} = 32(z-1)^4 (11z-4) z^4 - 32(z-1)^3 (6z+5) \eta z^3 - 4(z-1)^2 (12z-5) \eta^2 z^2 + 24(z-1) \eta^3 z + 3\eta^4, \quad (7.65)$$

$$P_{98} = 16(z-1)^3 (3z+1) z^3 - 4(z-1)^2 (6z+5) \eta z^2 + 6(z-1) \eta^2 z + 3\eta^3. \quad (7.66)$$

The  $g_i(\eta, z)$  functions, defined in the ranges  $0 < z < \eta_-$  and  $\eta_+ < z < 1$ , are given by

$$g_0(\eta, z) = \frac{z-1}{z} \left[ \frac{64P_{100}}{45\eta^{3/2}z} (\eta - 4z(1-z))^{3/2} K_3 \left( \frac{z(1-z)}{\eta} \right) + \frac{64}{3} K_4 \left( \frac{z(1-z)}{\eta} \right) + \frac{32}{45z} (6\eta + 30z^2 - 5z) \ln^2 \left( \frac{z(1-z)}{\eta} \right) + \frac{64\zeta_2 (6\eta + 30z^2 - 35z)}{45z} - \frac{128P_{99}}{45\eta^2 z} \ln \left( \frac{z(1-z)}{\eta} \right) + \frac{256(z-1)}{45\eta} (3\eta + 24z^2 - 34z) \right], \quad (7.67)$$

$$g_1(\eta, z) = -\frac{128P_{102}}{45\eta^{3/2}z^2} (\eta - 4z(1-z))^{3/2} K_3 \left( \frac{z(1-z)}{\eta} \right) - \frac{64P_{92}}{45z^2} \ln^2 \left( \frac{z(1-z)}{\eta} \right) - \frac{128(z-1)(4z+1)}{3z} K_4 \left( \frac{z(1-z)}{\eta} \right) + \frac{256P_{101}}{45\eta^2 z^2} \ln \left( \frac{z(1-z)}{\eta} \right) + \frac{256(z-1)}{45\eta z} (3\eta + 80z^3 - 36z^2 - 44z) + \frac{128\zeta_2 (3\eta + 20z^3 - 20z)}{45z^2}, \quad (7.68)$$

$$g_2(\eta, z) = \frac{256}{3} (z-1) \left[ \frac{2(\eta - 4z(1-z))^{3/2}}{3\eta^{3/2}} K_3 \left( \frac{z(1-z)}{\eta} \right) + 2K_4 \left( \frac{z(1-z)}{\eta} \right) - \frac{4}{3\eta^2} (-\eta + 4z^2 - 4z)^2 \ln \left( \frac{z(1-z)}{\eta} \right) - \frac{16(z-1)z}{3\eta} - \frac{2\zeta_2}{3} + \frac{5}{3} \ln^2 \left( \frac{z(1-z)}{\eta} \right) \right], \quad (7.69)$$

$$g_3(\eta, z) = \frac{64(z-1)}{z} \left[ \frac{2P_{104}}{9\eta^{3/2}} \sqrt{\eta - 4z(1-z)} K_3 \left( \frac{z(1-z)}{\eta} \right) + \frac{2}{3} K_4 \left( \frac{z(1-z)}{\eta} \right) - \frac{2P_{103}}{9\eta^2} \ln \left( \frac{z(1-z)}{\eta} \right) + \frac{8z}{27\eta} (-7\eta + 36z^2 - 42z + 6) + \frac{2}{9} (3z-1) \zeta_2 + \frac{1}{9} (3z+5) \ln^2 \left( \frac{z(1-z)}{\eta} \right) \right]. \quad (7.70)$$

Here the functions  $K_3$  and  $K_4$  are

$$K_3(u) = G \left( \left\{ \frac{1}{\tau}, \frac{\sqrt{1-4\tau}}{\tau} \right\}, u \right) - (\ln(u) + 2) G \left( \left\{ \frac{\sqrt{1-4\tau}}{\tau} \right\}, u \right) + \zeta_2, \quad (7.71)$$

$$K_4(u) = -G \left( \left\{ \frac{\sqrt{1-4\tau}}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau} \right\}, u \right) + \zeta_2 G \left( \left\{ \frac{\sqrt{1-4\tau}}{\tau} \right\}, u \right)$$

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$$-2G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}\right\}, u\right) + \zeta_2 \ln(u) + \frac{1}{6} \ln^3(u), \quad (7.72)$$

and

$$P_{99} = 16(z-1)^2(6z-1)z^3 - 8(z-1)(9z-4)\eta z^2 - (36z-41)\eta^2 z - 6\eta^3, \quad (7.73)$$

$$P_{100} = z(6z-1) - 6\eta, \quad (7.74)$$

$$P_{101} = 32(z-1)^3(10z+1)z^3 - 4(z-1)^2(40z+1)\eta z^2 + (z-1)(20z+23)\eta^2 z + 3\eta^3, \quad (7.75)$$

$$P_{102} = 2(z-1)z(10z+1) + 3\eta, \quad (7.76)$$

$$P_{103} = 32(z-1)^2(3z+1)z^2 - 16(z-1)(3z+1)\eta z + (2-7z)\eta^2, \quad (7.77)$$

$$P_{104} = 4(z-1)z(3z+1) + (1-6z)\eta. \quad (7.78)$$

Finally, the  $h_i(\eta, z)$  functions, defined in the full range  $0 < z < 1$ , are just given by the  $g_i(\eta, z)$  functions with  $\eta \rightarrow 1/\eta$ , i.e.,

$$h_i(\eta, z) = g_i\left(\frac{1}{\eta}, z\right), \quad i = 0, 1, 2, 3. \quad (7.79)$$

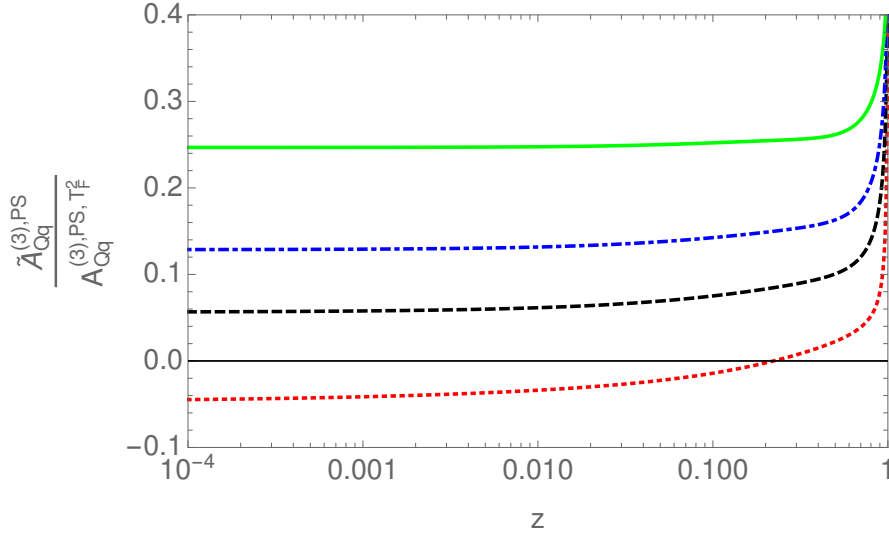


Figure 7.3.: The ratio of the 2-mass contributions to the massive OME  $\tilde{A}_{Qq}^{\text{PS},(3)}$  to all contributions to  $A_{Qq}^{\text{PS},(3)}$  of  $\mathcal{O}(T_F^2)$  as a function of  $z$  and  $\mu^2$ . Dotted line (red):  $\mu^2 = 30 \text{ GeV}^2$ . Dashed line (black):  $\mu^2 = 50 \text{ GeV}^2$ . Dash-dotted line (blue):  $\mu^2 = 100 \text{ GeV}^2$ . Full line (green):  $\mu^2 = 1000 \text{ GeV}^2$ . Here the on-shell heavy quark masses  $m_c = 1.59 \text{ GeV}$  and  $m_b = 4.78 \text{ GeV}$  [208, 357] have been used.

We see that iterated integrals of up to weight three appear in our result. The alphabet of these integrals is given in terms of just three letters:

$$\frac{1}{\tau}, \quad \sqrt{4-\tau}\sqrt{\tau}, \quad \frac{\sqrt{1-4\tau}}{\tau}. \quad (7.80)$$

In principle, we could try to calculate all of the integrals in  $y$  appearing in Eq. (7.44) and express them in terms of iterated integrals of higher weight. However, this is not really necessary or even convenient, since the expressions (7.48–7.51, 7.67–7.68) are very compact, and integrating them into higher weight

iterated integrals leads to a result of considerably larger size. Furthermore, all of the iterated integrals appearing above can be written in terms of simple polylogarithms (albeit of complicated arguments), cf. Appendix H.1, for which various fast converging numerical representations exist. Therefore, the integrals in  $y$  appearing in Eq. (7.44) can be performed numerically without problems. The convolution with parton distribution functions, in order to compute the corresponding contribution to  $F_2(x, Q^2)$  or for the transition rate in the VNFS, is straightforward.

### 7.1.3. Numerical Results

We compare the pure singlet two-mass contributions to the complete  $\mathcal{O}(T_F^2)$  term as a function of  $z$  and  $\mu^2$  in Figure 7.3. Typical virtualities are  $\mu^2 \in [30, 1000]$  GeV<sup>2</sup>. The ratio of the 2-mass contributions to the complete term of  $\mathcal{O}(T_F^2)$  grows in this region from slightly negative contributions to  $\sim 0.36$  for very large virtualities in most of the  $z$ -range. The behavior of the ratio is widely flat in  $z$ , rising at very large  $z$ .

## 7.2. The Gluonic Operator Matrix Element $A_{gg,Q}^{(3)}$

There are 76 diagrams contributing to the irreducible part of  $\tilde{A}_{gg,Q}^{(3)}$ . With symmetry arguments these can be reduced to the 12 topologies shown in Fig. 7.4. The diagrams 1, 2, 3, 7, 9, 10 and 12 are symmetric under the exchange of the two masses, while the remaining ones have to be computed for both mass assignments. In principle we could also get the result for the other diagram by analytic continuation in  $\eta \rightarrow 1/\eta$ . However we chose to calculate all diagrams for both mass assignments and use their symmetry relations as an additional check on our calculation. In Ref. [202] the scalar prototypes of the diagrams have been computed first in  $z$ -space, similar to the approach of calculating the two mass contributions to the pure singlet OME. Subsequently, it was possible to Mellin transform the  $z$ -space result and arrive at the  $N$ -space solution since all difference equations were first order factorizable. Since the gluonic OME contains also contributions from the  $\delta$ - and  $+$ -distribution the integrals have to be performed very carefully, which is only hardly automatized. For the physical diagrams this is a serious problem since gluonic Feynman rules, cf. Chapter B, lead to large numerators and therefore to a large number of integrals which have to be solved. The sheer amount of integrals which have to be solved this way renders this approach of calculation unfeasible in the physical case. Therefore the order in which the two results are obtained is reversed for the physical diagrams. First the  $N$ -space solution is calculated and in the end the momentum space solution is obtained via an inverse Mellin transformation. This approach is highly automated and therefore suited to tackle this large scale problem. In order to check the feasibility of this approach we recalculated all of the scalar diagrams and found agreement.

The first steps are similar to the pure singlet case. After generating the 76 diagrams using QGRAF [362] and identifying the 12 different topologies, dedicated FORM [198] routines were set up to perform the Dirac algebra and traces. The color algebra is done using the FORM program COLOR [363]. For fermionic bubble insertions we use the identity

$$\Pi_{ab}^{\mu\nu}(k) = -\frac{8T_F g^2}{(4\pi)^{d/2}} \delta_{ab} (k^2 g^{\mu\nu} - k^\mu k^\nu) \int_0^1 dx \frac{\Gamma(2-d/2) (x(1-x))^{d/2-1}}{\left(-k^2 + \frac{m^2}{x(1-x)}\right)^{2-d/2}}, \quad (7.81)$$

instead of the Mellin-Barnes integral representation given in Eq. (7.2). This will allow to derive contour integrals which are easier to handle in an automated way.

In the next step the Feynman parametrization, was performed on the full numerator and denominator structure, i.e. no cancelation between numerator and denominator was performed. This allows a uniform Feynman parametrization for the whole diagram, also resulting in less special cases and

## 7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

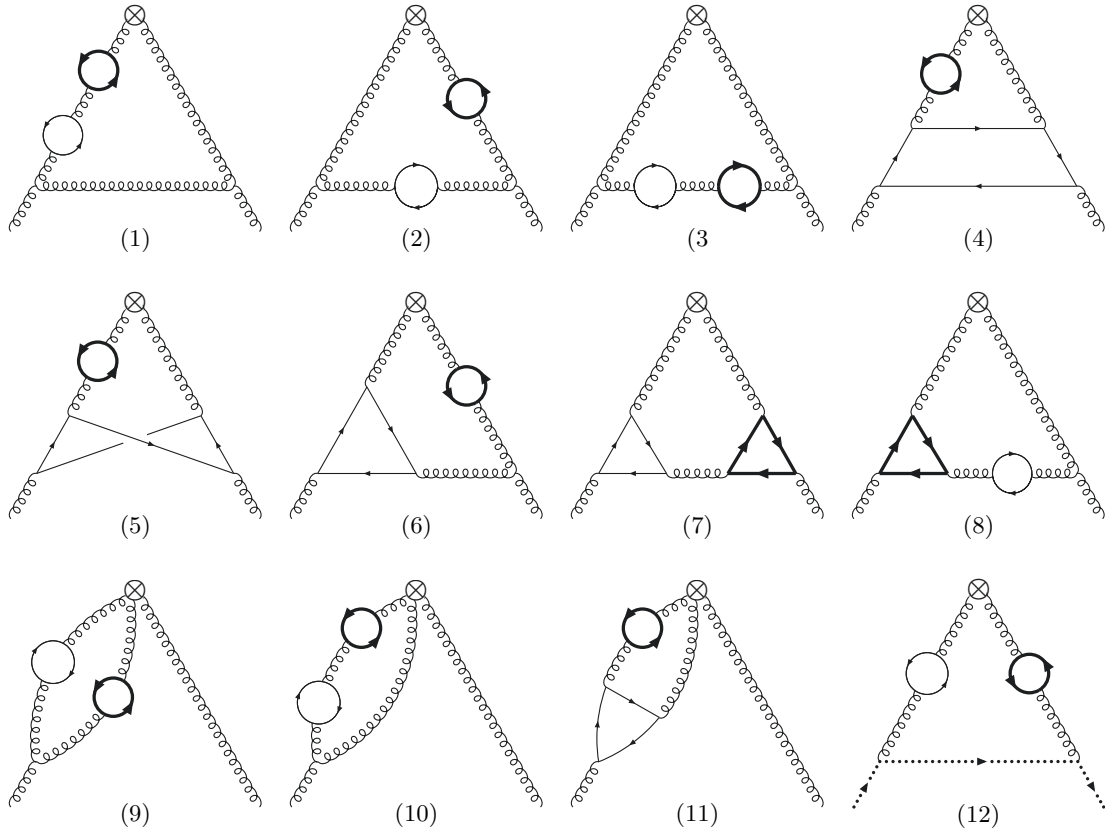


Figure 7.4.: The twelve different topologies for  $\tilde{A}_{gg,Q}^{(3)}$ . Curly lines: gluons; dotted lines: ghosts; thin arrow lines: lighter massive quark; thick arrow lines: heavier massive quark; the symbol  $\otimes$  represents the corresponding local operator insertion, cf. [182].

complexity for the subsequent calculation. The resulting tensor integrals were reduced to scalar ones according to the rules stated in Appendix G and thus mapped to the basic one-loop integral in Eq. (G.8). It is important to perform the integration of the momentum with the operator insertion as the last one. In this way only the additional scalar product  $p \cdot k$  can appear, which simplifies the reduction to scalar integrals drastically, since only a single term of the binomial decomposition of  $(k \cdot \Delta + R_0 p \cdot \Delta)^N$  can contribute to the integral.

After these steps we are left with a linear combination of up to 7-fold Feynman parameter integrals, with the general structure

$$\prod_{j=1}^i \int_0^1 dx_i x_i^{a_i} (1-x_i)^{b_i} R_0^N [R_1 m_a^2 + R_2 m_b^2]^{-s}. \quad (7.82)$$

Here  $R_1$  and  $R_2$  are simple rational functions of  $x_i$  and  $1-x_i$  and  $R_0$  is a polynomial in  $x_i$  stemming from the local operator insertion. In the next step we split the rightmost factor by means of a Mellin-Barnes integral [188–191]

$$\frac{1}{(A+B)^s} = \frac{1}{2\pi i} \frac{1}{\Gamma(s)} B^{-s} \int_{-i\infty}^{+i\infty} d\sigma \left(\frac{A}{B}\right)^\sigma \Gamma(-\sigma) \Gamma(\sigma+s), \quad (7.83)$$

where the real part of the integration contour has to be chosen such that the ascending poles are separated from the descending ones. Our next aim is to compute the Feynman parameter integrals.

To do this, the operator polynomial  $R_0$  can be decomposed with the help of the binomial theorem

$$(A + B)^N = \sum_{i=0}^N \binom{N}{i} A^i B^{N-i}. \quad (7.84)$$

This splitting has to be performed as often as necessary to obtain hyperexponential terms in  $x_i$  and  $1 - x_i$  only. In the present case, we had to split the polynomial up to three times. Attempts to combine the expression into a linear combination of higher transcendental functions in order to keep the additional summations as few as possible have failed, because overlapping divergencies of the  $\Gamma$ -functions appeared, preventing to choose a proper path for the Mellin-Barnes integral. This indicates that these transformations cannot be performed naively after the Mellin-Barnes representation has been applied. Applying these transformations, all Feynman parameter integrals can be expressed by Euler's Beta-functions

$$B(a, b) = \int_0^1 dz z^{a-1} (1-z)^{b-1} = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}. \quad (7.85)$$

For example, we encountered the integral

$$\begin{aligned} I &= \Gamma\left(-\frac{3\varepsilon}{2}\right) \int_0^1 \left( \prod_{i=1}^7 dz_i \right) z_1^2 (z_2(1-z_2))^{\frac{\varepsilon}{2}} z_3^2 (z_4(1-z_4))^{\frac{\varepsilon}{2}} (1-z_5) (z_6(1-z_6))^{\frac{\varepsilon}{2}} z_7^{1+\frac{\varepsilon}{2}} \\ &\quad \times (1-z_7)^2 (z_7(z_1 z_6 + z_3(1-z_6)) + z_5(1-z_7))^{N-4} \left( \frac{z_6 m_a^2}{z_2(1-z_2)} + \frac{(1-z_6) m_b^2}{z_4(1-z_4)} \right)^{\frac{3\varepsilon}{2}} \end{aligned} \quad (7.86)$$

for the computation of diagram 7 in Figure 7.4. Here we can decompose the operator polynomial as

$$\begin{aligned} &(z_7(z_1 z_6 + z_3(1-z_6)) + z_5(1-z_7))^{N-4} = \\ &\quad \sum_{j=0}^{N-4} \sum_{i=0}^j \binom{N-4}{j} \binom{j}{i} z_7^j z_1^i z_6^i z_3^{j-i} (1-z_6)^{j-i} z_5^{N-4-j} (1-z_7)^{N-4-j}. \end{aligned} \quad (7.87)$$

After applying the Mellin-Barnes integral and integrating the Feynman parameters we find

$$\begin{aligned} I &= \frac{(m_b^2)^{\frac{3\varepsilon}{2}}}{2\pi i} \sum_{j=0}^{N-4} \sum_{i=0}^j \binom{N-4}{j} \binom{j}{i} \frac{\Gamma(3+i)\Gamma(3-i+j)\Gamma(N-j-3)}{\Gamma(4+i)\Gamma(4-i+j)\Gamma(N+1+\frac{\varepsilon}{2})} \int_{-i\infty}^{+i\infty} d\sigma \left( \frac{m_a^2}{m_b^2} \right)^\sigma \\ &\quad \times \Gamma(-\sigma)\Gamma(-\frac{3\varepsilon}{2} + \sigma)\Gamma(1 - \frac{\varepsilon}{2} + i + \sigma)\Gamma(1 + \varepsilon - i + j - \sigma) \\ &\quad \times \frac{\Gamma(1 + \frac{\varepsilon}{2} - \sigma)\Gamma(3 + \frac{\varepsilon}{2} - \sigma)\Gamma(1 - \varepsilon - \sigma)\Gamma(3 - \varepsilon + \sigma)}{\Gamma(4 + \varepsilon - 2\sigma)\Gamma(4 - 2\varepsilon + 2\sigma)}. \end{aligned} \quad (7.88)$$

Note that the summands arising from the binomial decomposition in Eq. (7.84) appear naturally in nested form. We have not yet specified  $m_a$  or  $m_b$  to the physical masses, since there are diagrams with both possibilities. In the following we choose to exploit the symmetry of the Mellin-Barnes integral to arrive at two different representations either proportional to  $(m_a^2/m_b^2)^\sigma$  or to  $(m_b^2/m_a^2)^\sigma$ . In this way we can choose  $m_a^2/m_b^2 = \eta$  or  $m_b^2/m_a^2 = \eta$  and close the contour to the right in both cases. At this point we could have followed earlier approaches by applying the packages `MB` [360] and `MBresolve` [361] to resolve the singularity structure of the integrals and expand the final integral in  $\varepsilon$ . However, the additional dependence on  $N$  and up to four summation quantifiers renders the automated finding of a suitable integration contour non-trivial. Therefore, we calculated these integrals by summing

up the residues of the ascending poles of the integrand keeping the  $\varepsilon$ -dependence and are expanding afterwards. In general, residues had to be taken at  $\sigma = k$ ,  $\sigma = k + \varepsilon/2$  and  $\sigma = k + \varepsilon$ , where  $k$  is an integer larger than an integral specific minimum. In the end, each integral is represented by a linear combination of three infinite sums, over which additional binomial sums have to be performed. Nevertheless, we used the packages `MB` and `MBresolve` to check our sum representations for fixed values of the Mellin variable  $N$ .

The final multi-sum can now be handled by the packages `Sigma` [268, 269], `EvaluateMultiSums` and `SumProduction` [271]. Here additionally `HarmonicSums` [240, 273, 275] was used for limiting procedures and operations on special functions and numbers. The sum representation of each integral, which can take up to  $\mathcal{O}(100\text{MB})$ , was crushed to an optimal representation using `SumProduction`. This representation contains constants from taking out points from summation boundaries and multi-sums with large summand structures. These multi-sums were then handled by `EvaluateMultiSums`, which uses `Sigma` and `HarmonicSums`. The results were expressed in terms of nested harmonic-, generalized harmonic-, cyclotomic- and binomial-sums. Furthermore, generalized harmonic- and cyclotomic-sums at infinity contribute. These can be expressed in terms of HPLs depending on  $\eta$  in the argument with the help of `HarmonicSums`. More information on the underlying mathematical and algorithmic details can be found in [2].

Prior to the solution for general values of  $N$ , our sum representations also allow to calculate fixed even moments, without expanding in the parameter  $\eta$ . They also serve as input values for the general  $N$ -solution.

### 7.2.1. An Explanatory Example

In this section the computational steps are described in more detail on the calculation of diagram 2 in Figure 7.4. Since here the  $\eta$  and  $N$  structures do not factorize, the result gives rise to more involved structures compared to the single mass case. However, the small numerator structure of this diagram allows to present the calculation in full detail.

After inserting the Feynman rules, applying the gluonic projector, performing the Dirac-algebra and combining the denominators via Feynman parameters, one obtains

$$\begin{aligned}
 D_2^{A(B)} = & -C_A T_F^2 \frac{1 + (-1)^N}{2} \frac{a_s^3}{(4\pi)^{3\varepsilon/2}} \frac{64}{2 + \varepsilon} \frac{1}{2\pi i} \left[ (10 + 4\varepsilon) J_1^{A(B)}(N - 1) + (2 + \varepsilon) J_1(N)^{A(B)} \right. \\
 & - 4(3 + \varepsilon) J_2^{A(B)}(N - 1) + 4(2 + \varepsilon) J_2^{A(B)}(N) + 2(5 + 2\varepsilon) J_2^{A(B)}(N - 2) \\
 & \left. + 2J_3^{A(B)}(N - 1) - (2 + \varepsilon) J_3^{A(B)}(N - 2) \right], \tag{7.89}
 \end{aligned}$$

where  $A(B)$  represent different mass assignments. The functions  $J_i$  are normalized according to

$$J_i^{A(B)}(n) = \left( \frac{m_1^2}{\mu^2} \right)^{\frac{3\varepsilon}{2}} j_i^{A(B)}(n). \tag{7.90}$$

In the following we use the notation introduced in (C.13) to abbreviate the ratios of  $\Gamma$  functions.

#### The $N$ -space solution

The functions  $J_1$  to  $J_3$  are given by the following expressions

$$\begin{aligned}
 j_1^A(n) &= \int_{-i\infty}^{+i\infty} d\sigma \eta^\sigma \Gamma \left[ \begin{matrix} -\sigma, \sigma - \frac{3\varepsilon}{2}, (2 + \frac{\varepsilon}{2} - \sigma)^2, (2 - \varepsilon + \sigma)^2, \varepsilon - \sigma, n - \frac{\varepsilon}{2} + \sigma \\ 4 + \varepsilon - 2\sigma, 4 - 2\varepsilon + 2\sigma, 2 + \varepsilon + n \end{matrix} \right], \\
 j_1^B(n) &= \int_{-i\infty}^{+i\infty} d\sigma \eta^\sigma \Gamma \left[ \begin{matrix} -\sigma, \sigma - \frac{3\varepsilon}{2}, \sigma - \frac{\varepsilon}{2}, (2 - \varepsilon + \sigma)^2, (2 + \frac{\varepsilon}{2} - \sigma)^2, n + \varepsilon - \sigma \\ 2 + n + \frac{\varepsilon}{2}, 4 + \varepsilon - 2\sigma, 4 - 2\varepsilon + 2\sigma \end{matrix} \right],
 \end{aligned}$$

$$\begin{aligned}
 j_2^A(n) &= \int_{-i\infty}^{+i\infty} d\sigma \eta^\sigma \Gamma \left[ -\sigma, \sigma - \frac{3\varepsilon}{2}, \varepsilon - \sigma, 1 - \frac{\varepsilon}{2} + n + \sigma, \sigma - \frac{\varepsilon}{2}, (2 - \varepsilon + \sigma)^2, (2 + \frac{\varepsilon}{2} - \sigma)^2 \right. \\
 &\quad \left. 4 + \varepsilon - 2\sigma, 4 - 2\varepsilon + 2\sigma, 1 - \frac{\varepsilon}{2} + \sigma, \frac{\varepsilon}{2} + 2 + n \right], \\
 j_2^B(n) &= \int_{-i\infty}^{+i\infty} d\sigma \eta^\sigma \Gamma \left[ -\sigma, \sigma - \frac{3\varepsilon}{2}, \sigma - \frac{\varepsilon}{2}, (2 - \varepsilon - \sigma)^2, (2 + \frac{\varepsilon}{2} - \sigma)^2, \varepsilon - \sigma, 1 + n + \varepsilon - \sigma \right. \\
 &\quad \left. 1 + \varepsilon - \sigma, 2 + n + \frac{\varepsilon}{2}, 4 + \varepsilon - 2\sigma, 4 - 2\varepsilon + 2\sigma \right], \\
 j_3^A(n) &= \int_{-i\infty}^{+i\infty} d\sigma \eta^\sigma \Gamma \left[ -\sigma, \sigma - \frac{3\varepsilon}{2}, \varepsilon - \sigma, (\frac{\varepsilon}{2} + 2 - \sigma)^2, (2 - \varepsilon + \sigma)^2, \sigma - \frac{\varepsilon}{2}, 2 - \frac{\varepsilon}{2} + n + \sigma \right. \\
 &\quad \left. \varepsilon + 4 - 2\sigma, -2\varepsilon + 4 + 2\sigma, \frac{\varepsilon}{2} + 2 + n, 2 - \frac{\varepsilon}{2} + \sigma \right], \\
 j_3^B(n) &= \int_{-i\infty}^{+i\infty} d\sigma \eta^\sigma \Gamma \left[ -\sigma, \sigma - \frac{3\varepsilon}{2}, \sigma - \frac{\varepsilon}{2}, (2 - \varepsilon + \sigma)^2, (2 + \frac{\varepsilon}{2} - \sigma)^2, \varepsilon - \sigma, 2 + n + \varepsilon - \sigma \right. \\
 &\quad \left. 2 + \varepsilon - \sigma, 2 + n + \frac{\varepsilon}{2}, 4 + \varepsilon - 2\sigma, 4 - 2\varepsilon + 2\sigma \right].
 \end{aligned} \tag{7.91}$$

The contour integrals are evaluated by taking residues at the ascending poles and are subsequently added up. One obtains

$$J_1^A(n) = \left( \frac{m_1^2}{\mu^2} \right)^{3\varepsilon/2} \sum_{k=0}^{\infty} \eta^k (T_{1,1}(n) + T_{1,2}(n) + T_{1,3}(n)), \tag{7.92}$$

$$J_2^A(n) = \left( \frac{m_1^2}{\mu^2} \right)^{3\varepsilon/2} \sum_{k=0}^{\infty} \eta^k (T_{2,1}(n) + T_{2,2}(n) + T_{2,3}(n)), \tag{7.93}$$

$$J_3^A(n) = \left( \frac{m_1^2}{\mu^2} \right)^{3\varepsilon/2} \sum_{k=0}^{\infty} \eta^k (T_{3,1}(n) + T_{3,2}(n) + T_{3,3}(n)), \tag{7.94}$$

where  $T_{i,1}$  follows from the residue at  $\sigma = k$ ,  $T_{i,2}$  from the residue at  $\sigma = \varepsilon + k$  and  $T_{i,3}$  from the residue at  $\sigma = \varepsilon/2 + 2 + k$ . The explicit expressions read

$$T_{1,1}(n) = \frac{2^\varepsilon \pi}{64} \Gamma \left[ -\frac{\varepsilon}{2} - 2, -\varepsilon, \frac{\varepsilon}{2} + 3, \varepsilon + 1, k - \frac{3\varepsilon}{2}, 2 - \varepsilon + k, k - \frac{\varepsilon}{2} - \frac{3}{2}, n - \frac{\varepsilon}{2} + k \right. \\ \left. -\frac{\varepsilon}{2} - \frac{5}{2}, \frac{\varepsilon}{2} + \frac{7}{2}, \frac{\varepsilon}{2} + n + 2, 1 + k, 1 - \varepsilon + k, \frac{5}{2} - \varepsilon + k, k - \frac{\varepsilon}{2} - 1 \right], \tag{7.95}$$

$$T_{1,2}(n) = \frac{2^\varepsilon \pi \eta^\varepsilon}{64} \Gamma \left[ 3 - \frac{\varepsilon}{2}, 1 - \varepsilon, \frac{\varepsilon}{2} - 2, \varepsilon, 2 + k, k - \frac{\varepsilon}{2}, k + \frac{\varepsilon}{2} - \frac{3}{2}, \frac{\varepsilon}{2} + n + k \right. \\ \left. \frac{7}{2} - \frac{\varepsilon}{2}, \frac{\varepsilon}{2} - \frac{5}{2}, \frac{\varepsilon}{2} + n + 2, 1 + k, \frac{5}{2} + k, \varepsilon + 1 + k, \frac{\varepsilon}{2} - 1 + k \right], \tag{7.96}$$

$$T_{1,3}(n) = -\frac{2^\varepsilon \eta^{\frac{\varepsilon}{2}+2}}{64} \Gamma \left[ -\frac{\varepsilon}{2} - 1, 2 - \frac{\varepsilon}{2}, \frac{\varepsilon}{2} - 1, \frac{\varepsilon}{2} + 2, \frac{1}{2} + k, 2 + n + k, 2 - \varepsilon + k, 4 - \frac{\varepsilon}{2} + k \right. \\ \left. \frac{\varepsilon}{2} + 2 + n, 1 + k, 3 - \frac{\varepsilon}{2} + k, \frac{9}{2} - \frac{\varepsilon}{2} + k, \frac{\varepsilon}{2} + 3 + k \right], \tag{7.97}$$

$$T_{2,1}(n) = \frac{2^\varepsilon \pi}{64} \Gamma \left[ -2 - \frac{\varepsilon}{2}, 3 + \frac{\varepsilon}{2}, -\varepsilon, 1 + \varepsilon \right] \\ \times \Gamma \left[ k - \frac{3\varepsilon}{2}, 2 - \varepsilon + k, k - \frac{3}{2} - \frac{\varepsilon}{2}, k - \frac{\varepsilon}{2}, 1 + n - \frac{\varepsilon}{2} + k \right. \\ \left. 1 + k, 1 - \varepsilon + k, \frac{5}{2} - \varepsilon + k, k - 1 - \frac{\varepsilon}{2}, 1 - \frac{\varepsilon}{2} + k \right], \tag{7.98}$$

$$T_{2,2}(n) = \frac{2^\varepsilon \pi \eta^\varepsilon}{64} \Gamma \left[ 1 - \varepsilon, 3 - \frac{\varepsilon}{2}, \frac{\varepsilon}{2} - 2, \varepsilon \right] \\ \times \Gamma \left[ 2 + k, k - \frac{\varepsilon}{2}, \frac{\varepsilon}{2} - \frac{3}{2} + k, \frac{\varepsilon}{2} + k, 1 + n + \frac{\varepsilon}{2} + k \right. \\ \left. 1 + k, \frac{5}{2} + k, \frac{\varepsilon}{2} - 1 + k, 1 + \frac{\varepsilon}{2} + k, 1 + \varepsilon + k \right], \tag{7.99}$$

$$T_{2,3}(n) = -\frac{2^\varepsilon \eta^{\frac{\varepsilon}{2}+2}}{64} \Gamma \left[ -1 - \frac{\varepsilon}{2}, 2 - \frac{\varepsilon}{2}, 2 + \frac{\varepsilon}{2}, -1 + \frac{\varepsilon}{2} \right] \\ \left. 2 + n + \frac{\varepsilon}{2} \right]$$

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$$\times \Gamma \left[ \begin{matrix} \frac{1}{2} + k, 2 + k, 3 + n + k, 2 - \varepsilon + k, 4 - \frac{\varepsilon}{2} + k \\ 1 + k, 3 + k, 3 - \frac{\varepsilon}{2} + k, \frac{9}{2} - \frac{\varepsilon}{2} + k, 3 + \frac{\varepsilon}{2} + k \end{matrix} \right], \quad (7.100)$$

$$T_{3,1}(n) = \frac{2^\varepsilon \pi}{64} \Gamma \left[ \begin{matrix} -2 - \frac{\varepsilon}{2}, 3 + \frac{\varepsilon}{2}, -\varepsilon, 1 + \varepsilon \\ -\frac{5}{2} - \frac{\varepsilon}{2}, \frac{7}{2} + \frac{\varepsilon}{2}, 2 + n + \frac{\varepsilon}{2} \end{matrix} \right] \\ \times \Gamma \left[ \begin{matrix} k - \frac{3\varepsilon}{2}, 2 - \varepsilon + k, k - \frac{3}{2} - \frac{\varepsilon}{2}, k - \frac{\varepsilon}{2}, 2 + n - \frac{\varepsilon}{2} + k \\ 1 + k, 1 - \varepsilon + k, \frac{5}{2} - \varepsilon + k, k - 1 - \frac{\varepsilon}{2}, 2 - \frac{\varepsilon}{2} + k \end{matrix} \right], \quad (7.101)$$

$$T_{3,2}(n) = \frac{2^\varepsilon \pi \eta^\varepsilon}{64} \Gamma \left[ \begin{matrix} 1 - \varepsilon, 3 - \frac{\varepsilon}{2}, \frac{\varepsilon}{2} - 2, \varepsilon \\ \frac{7}{2} - \frac{\varepsilon}{2}, \frac{\varepsilon}{2} - \frac{5}{2}, 2 + n + \frac{\varepsilon}{2} \end{matrix} \right] \\ \times \Gamma \left[ \begin{matrix} 2 + k, k - \frac{\varepsilon}{2}, \frac{\varepsilon}{2} - \frac{3}{2} + k, \frac{\varepsilon}{2} + k, 2 + n + \frac{\varepsilon}{2} + k \\ 1 + k, \frac{5}{2} + k, \frac{\varepsilon}{2} - 1 + k, 2 + \frac{\varepsilon}{2} + k, 1 + \varepsilon + k \end{matrix} \right], \quad (7.102)$$

$$T_{3,3}(n) = -\frac{2^\varepsilon \eta^{\frac{\varepsilon}{2}+2}}{64} \Gamma \left[ \begin{matrix} -1 - \frac{\varepsilon}{2}, 2 - \frac{\varepsilon}{2}, \frac{\varepsilon}{2} - 1, 2 + \frac{\varepsilon}{2} \\ 2 + n + \frac{\varepsilon}{2} \end{matrix} \right] \\ \times \Gamma \left[ \begin{matrix} \frac{1}{2} + k, 2 + k, 4 + n + k, 2 - \varepsilon + k, 4 - \frac{\varepsilon}{2} + k \\ 1 + k, 4 + k, 3 - \frac{\varepsilon}{2} + k, \frac{9}{2} - \frac{\varepsilon}{2} + k, 3 + \frac{\varepsilon}{2} + k \end{matrix} \right]. \quad (7.103)$$

Here Legendre's duplication, cf. (C.10), and Euler's reflection formula, cf. (C.9) were used to simplify the  $\Gamma$ -ratios.

In the following the focus will be on the calculation of  $D_2^A$ . The expressions for  $J_i^B$  needed for the evaluation of  $D_2^B$  look similar. It is worth mentioning, however, that care is needed at taking the residues for the other mass assignment. Here structures like

$$\frac{\Gamma(\varepsilon - \sigma)\Gamma(2 + n + \varepsilon - \sigma)}{\Gamma(2 + \varepsilon - \sigma)} \quad (7.104)$$

develop residues at isolated boundary points, i.e. in this example the residues at  $\sigma = \varepsilon, 1 + \varepsilon$  have to be treated differently than the ones at  $\sigma = 2 + n + \varepsilon + k$  with  $k \in \mathbb{N}$ . Therefore, the final representation for  $D_2^B$  does not only contain sums but also terms from residues taken separately.

The full expression for  $D_2^A$  can now be handled with `SumProduction`, `EvaluateMultiSums`, `Sigma` and `HarmonicSums`. For the complete diagram we obtain

$$D_2^A = C_A T_F^2 \frac{1 + (-1)^N}{2} a_s^3 S_\varepsilon^3 \left( \frac{m_1^2}{\mu^2} \right)^{\frac{3\varepsilon}{2}} \left\{ \frac{256 P_{112}}{27 \varepsilon^3 (N-1)N(N+1)} + \frac{1}{\varepsilon^2} \left[ \frac{64 P_{108}}{81 (N-1)^2 N^2 (N+1)^2} \right. \right. \\ + \frac{64 P_{112}}{9 (N-1)N(N+1)} H_0(\eta) - \frac{64 P_{112}}{27 (N-1)N(N+1)} S_1 \left. \right] + \frac{1}{\varepsilon} \left[ \frac{32 P_{110}}{81 (N-1)^3 N^3 (N+1)^3} \right. \\ + \frac{32 P_{107}}{27 (N-1)^2 N^2 (N+1)^2} H_0(\eta) + \frac{32 P_{112}}{9 (N-1)N(N+1)} H_0^2(\eta) \\ - \frac{32 P_{109}}{81 (N-1)^2 N^2 (N+1)^2} S_1 + \frac{32 P_{112}}{27 (N-1)N(N+1)} S_1^2 + \left. \frac{32 P_{112}}{9 (N-1)N(N+1)} \zeta_2 \right] \\ - \frac{8 P_{115}}{729 (N-1)^4 N^4 (N+1)^4 (2N-5)(2N-3)(2N-1)\eta} \\ + \frac{2 P_{111} (1-\eta)^{-N}}{27 (N-1)^2 N^2 (N+1)(2N-5)(2N-3)(2N-1)\eta} \left( \frac{1}{2} H_0(\eta)^2 \right. \\ \left. + H_0(\eta) S_1(1-\eta, N) - S_2(1-\eta, N) + S_{1,1}(1-\eta, 1, N) \right) \\ - \frac{4 P_{113}}{27 (N-1)^3 N^3 (N+1)^3 (2N-5)(2N-3)(2N-1)\eta} H_0(\eta) \\ \left. + \frac{8 P_{106}}{27 (N-1)^2 N^2 (N+1)^2} H_0^2(\eta) + \frac{32 P_{112}}{27 (N-1)N(N+1)} H_0^3(\eta) \right\}$$



$$\begin{aligned}
 & -\frac{8P_{112}}{9(N-1)N(N+1)}H_0^2(\eta)H_1(\eta) + \frac{16P_{112}}{9(N-1)N(N+1)}H_0(\eta)H_{0,1}(\eta) \\
 & -\frac{16P_{112}}{9(N-1)N(N+1)}H_{0,0,1}(\eta) + \left( \frac{8P_{112}}{9(N-1)N(N+1)}H_0^2(\eta) \right. \\
 & -\frac{16P_{105}}{9(N-1)^2N^2(N+1)}H_0(\eta) - \frac{4P_{114}}{81(N-1)^3N^3(N+1)^3(2N-5)(2N-3)(2N-1)\eta} \\
 & \left. -\frac{8P_{112}}{9(N-1)N(N+1)}S_2 \right) S_1 + \left( \frac{8P_{108}}{81(N-1)^2N^2(N+1)^2} \right. \\
 & +\frac{8P_{112}}{9(N-1)N(N+1)}H_0(\eta) \left. \right) S_1^2 - \frac{8P_{112}}{81(N-1)N(N+1)}S_1^3 + \left( \frac{8P_{105}}{9(N-1)^2N^2(N+1)} \right. \\
 & +\frac{8P_{112}}{9(N-1)N(N+1)}H_0(\eta) \left. \right) S_2 - \frac{112P_{112}}{81(N-1)N(N+1)}S_3 \\
 & -\frac{16P_{112}}{9(N-1)N(N+1)}\left( \frac{1}{2}H_0^2(\eta) + S_{1,1}(1-\eta, 1, N) \right) S_1\left( \frac{1}{1-\eta}, N \right) \\
 & -\frac{16P_{112}}{9(N-1)N(N+1)}\left( H_0(\eta)S_{1,1}\left( \frac{1}{1-\eta}, 1-\eta, N \right) - S_{1,2}\left( \frac{1}{1-\eta}, 1-\eta, N \right) \right. \\
 & \left. +S_{1,2}\left( 1-\eta, \frac{1}{1-\eta}, N \right) - S_{1,1,1}\left( 1-\eta, 1, \frac{1}{1-\eta}, N \right) - S_{1,1,1}\left( 1-\eta, \frac{1}{1-\eta}, 1, N \right) \right) \\
 & -\frac{4^{-N}P_{116}}{54\eta^{3/2}(N+1)(2N-5)(2N-3)(2N-1)}\binom{2N}{N}\left( H_0^2(\eta)[H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})] \right. \\
 & \left. -4H_0(\eta)[H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta})] + 8[H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta})] \right) \\
 & -\frac{4^{-N}P_{116}}{27(N+1)(2N-5)(2N-3)(2N-1)\eta}\binom{2N}{N}\sum_{i=1}^N\frac{4^i}{\binom{2i}{i}}\left( \frac{1}{i^3} - \frac{1}{i^2}H_0(\eta) - \frac{1}{i^2}S_1(i) \right. \\
 & \left. +\frac{(1-\eta)^{-i}}{i}\left[ \frac{1}{2}H_0^2(\eta) + S_1(1-\eta, i)H_0(\eta) - S_2(1-\eta, i) + S_{1,1}(1-\eta, 1, i) \right] \right) \\
 & +\left( \frac{8P_{108}}{27(N-1)^2N^2(N+1)^2} + \frac{8P_{112}}{3(N-1)N(N+1)}H_0(\eta) - \frac{8P_{112}}{9(N-1)N(N+1)}S_1 \right) \zeta_2 \\
 & -\frac{32P_{112}}{27(N-1)N(N+1)}\zeta_3 \left. \right\}, \tag{7.105}
 \end{aligned}$$

with the polynomials

$$P_{105} = N^5 - N^4 + 2N^3 - 14N^2 - 4N + 6, \tag{7.106}$$

$$P_{106} = N^6 - 36N^5 - 33N^4 + 12N^3 + 224N^2 + 66N - 54, \tag{7.107}$$

$$P_{107} = 2N^6 - 18N^5 - 15N^4 - 12N^3 + 85N^2 + 36N - 18, \tag{7.108}$$

$$P_{108} = 7N^6 - 36N^5 - 27N^4 - 60N^3 + 116N^2 + 78N - 18, \tag{7.109}$$

$$P_{109} = 8N^6 - 18N^5 - 9N^4 - 84N^3 - 23N^2 + 48N + 18, \tag{7.110}$$

$$P_{110} = 30N^9 - 94N^8 - 112N^7 - 43N^6 + 300N^5 + 56N^4 - 272N^3 - 99N^2 + 30N - 36, \tag{7.111}$$

$$\begin{aligned}
 P_{111} = & -8N^9\eta^2 - 4N^8\eta(28 - 23\eta) - 2N^7(15 - 566\eta + 87\eta^2) + 3N^6(35 - 1162\eta - 185\eta^2) \\
 & -2N^5(30 - 1605\eta - 1099\eta^2) - 4N^4(75 - 367\eta + 608\eta^2) + 2N^3(255 + 127\eta + 12\eta^2) \\
 & -45N^2(5 + 202\eta - 35\eta^2) + 8064N\eta - 2160\eta, \tag{7.112}
 \end{aligned}$$

$$P_{112} = N^3 - 3N^2 - 2N - 6, \tag{7.113}$$

$$\begin{aligned}
 P_{113} = & 8N^{13}\eta^2 - 12N^{12}\eta(46 + 7\eta) - 2N^{11}(15 - 1970\eta - 37\eta^2) + N^{10}(75 - 7772\eta + 813\eta^2) \\
 & +3N^9(25 + 298\eta - 575\eta^2) - N^8(435 - 2834\eta + 495\eta^2) + N^7(165 + 19500\eta + 3511\eta^2)
 \end{aligned}$$

## 7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

$$\begin{aligned}
& +N^6(645 - 26320\eta - 1833\eta^2) - N^5(435 + 9526\eta + 1823\eta^2) \\
& -N^4(285 - 23566\eta - 2679\eta^2) + 15N^3(15 + 40\eta - 3\eta^2) - 36N^2\eta(281 + 30\eta) \\
& +5472N\eta - 1080\eta, \tag{7.114}
\end{aligned}$$

$$\begin{aligned}
P_{114} = & 24N^{13}\eta^2 + 12N^{12}(22 - 21\eta)\eta - 2N^{11}(45 + 1418\eta - 111\eta^2) \\
& +N^{10}(225 + 7628\eta + 2439\eta^2) + 3N^9(75 - 2002\eta - 1725\eta^2) \\
& -5N^8(261 - 2030\eta + 297\eta^2) + 3N^7(165 - 8900\eta + 3511\eta^2) \\
& +N^6(1935 + 3064\eta - 5499\eta^2) - N^5(1305 - 28030\eta + 5469\eta^2) \\
& -N^4(855 + 5686\eta - 8037\eta^2) + 3N^3(225 - 4312\eta - 45\eta^2) \\
& +60N^2\eta(49 - 54\eta) - 432N\eta + 1080\eta, \tag{7.115}
\end{aligned}$$

$$\begin{aligned}
P_{115} = & 216N^{16}\eta^2 - 4N^{15}\eta(836 + 567\eta) + 6N^{14}(135 + 6466\eta + 297\eta^2) \\
& -3N^{13}(675 + 34454\eta - 8073\eta^2) - 3N^{12}(945 - 11644\eta + 16191\eta^2) \\
& +2N^{11}(6885 - 8819\eta - 17658\eta^2) - 6N^{10}(405 - 72572\eta - 23562\eta^2) \\
& -2N^9(14580 + 147371\eta + 14418\eta^2) + 6N^8(2700 - 111523\eta - 24003\eta^2) \\
& +162N^7(155 + 3061\eta + 527\eta^2) - 6N^6(2970 - 92344\eta - 5571\eta^2) \\
& -N^5(7695 + 547820\eta + 50463\eta^2) + 3N^4(2025 + 7994\eta + 10125\eta^2) \\
& +90N^3\eta(730 + 81\eta) - 108N^2\eta(526 + 135\eta) + 35964N\eta - 4860\eta, \tag{7.116}
\end{aligned}$$

$$\begin{aligned}
P_{116} = & -16N^6\eta^3 - 72N^5\eta^2(3 - 2\eta) - 12N^4\eta(27 - 135\eta - 4\eta^2) \\
& -6N^3(5 - 270\eta + 351\eta^2 + 222\eta^3) + N^2(45 - 2349\eta - 2673\eta^2 + 1129\eta^3) \\
& +12N(5 + 216\eta + 72\eta^2 + 77\eta^3) - 45(1 - \eta)(5 + 104\eta - 13\eta^2). \tag{7.117}
\end{aligned}$$

The diagram explicitly fulfills the symmetry

$$D_2^A(m_1, m_2, \eta) = D_2^B\left(m_2, m_1, \frac{1}{\eta}\right). \tag{7.118}$$

All diagrams which differ for the two possible mass assignments have been calculated separately and the symmetry relation has been checked analytically. For mass symmetric diagrams, the independence of the mass assignment has been checked explicitly.

### The $z$ -space solution

The OME  $A_{gg,Q}$  receives contributions from distributions. The  $z$ -space result of diagram 2A can therefore be split into three parts. A regular part, a part to be understood as  $+$ -distribution and a part proportional to the  $\delta$ -distribution. An algorithm to find the inverse Mellin transform from the result given in the previous section has been presented in [364, 365] and is implemented in the package `HarmonicSums`. The general idea is to derive a differential equations for the  $z$ -space solution starting from a  $N$ -space recurrence which can be easily obtained from the analytic  $N$ -space result. Subsequently the differential equations can be solved. To tackle the problem at hand various optimizations had to be included.

Using these new algorithms the result in  $z$ -space for diagram 2A, split into the above mentioned three parts, reads:

$$\begin{aligned}
D_2^A(z) = & C_{AT_F^2} \frac{1 + (-1)^N}{2} \left[ D_2^{A,\delta} \delta(1 - z) + D_2^{A,+}(z) + D_2^{A,\text{reg}}(z) + M^{-1} [(N - 1)g_1(N - 1)](z) \right. \\
& \left. + M^{-1} [(N - 1)^2 g_2(N - 1)](z) \right], \tag{7.119}
\end{aligned}$$

where  $M^{-1}$  denotes the inverse Mellin transform. Terms of the type

$$M^{-1} \left[ (N - 1)^l g_l(N - 1) \right](z), \quad l = 1, 2, \tag{7.120}$$

which will not contribute in the sum of all diagrams are dropped in the following expressions. The rational pre-factors can be absorbed by applying the relations

$$\frac{1}{(N-1+a)^i} \int_0^1 dz z^{N-1} f(z) = \int_0^1 dz z^{N-1} \left\{ \int_z^1 dy \frac{(-1)^{i-1}}{(i-1)!} \left(\frac{y}{z}\right)^a \left[ \mathbf{H}_0\left(\frac{y}{z}\right) \right]^{i-1} f(y) \right\} \quad (7.121)$$

$$(N-1) \int_0^1 dz z^{N-1} f(z) = (z^{N-1} - 1)zf(z)|_0^1 - \int_0^1 (z^{N-1} - 1) \frac{d}{dz} (zf(z)). \quad (7.122)$$

In the following the renormalization scale is identified with the mass  $\mu = m_1$  and only the terms proportional to  $\varepsilon^0$  will be given for brevity. The logarithmic dependence on the mass can be easily restored by using the full  $N$ -space result and will be entirely given in terms of harmonic polylogarithms. One obtains

$$D_2^{A,\delta,\varepsilon^0} \propto \frac{4}{729}(836 + 243\eta) + \frac{2}{9}(46 + 3\eta)\mathbf{H}_0(\eta) + \frac{8}{27}\mathbf{H}_0^2(\eta) + \frac{32}{27}\mathbf{H}_0^3(\eta) - \frac{8}{9}\mathbf{H}_0^2(\eta)\mathbf{H}_1(\eta) + \frac{16}{9}\mathbf{H}_0(\eta)\mathbf{H}_{0,1}(\eta) - \frac{16}{9}\mathbf{H}_{0,0,1}(\eta) + \frac{8}{27}(7 + 9\mathbf{H}_0(\eta))\zeta_2 - \frac{32}{27}\zeta_3, \quad (7.123)$$

$$D_2^{A,+,\varepsilon^0}(z) \propto \frac{1}{1-z} \left[ \frac{2}{27}(22 - 9\eta) + \frac{16}{9}\mathbf{H}_0(\eta) - \frac{8}{9}\mathbf{H}_0^2(\eta) + \frac{16}{81}\mathbf{H}_0 + \frac{8}{27}\mathbf{H}_0^2 - \left( \frac{16}{27}\mathbf{H}_0 + \frac{16}{81}(7 + 9\mathbf{H}_0(\eta)) \right) \mathbf{H}_1 + \frac{8}{27}\mathbf{H}_1^2 + \frac{16}{9}\mathbf{H}_{0,1} \right] - \frac{(27 - 8\eta)\sqrt{\eta}}{108\pi(1-z)^{3/2}\sqrt{z}} \left[ \mathbf{H}_0^2(\eta) \left( \mathbf{H}_{-1}(\sqrt{\eta}) + \mathbf{H}_1(\sqrt{\eta}) \right) - 4\mathbf{H}_0(\eta) \left( \mathbf{H}_{0,1}(\sqrt{\eta}) + \mathbf{H}_{0,-1}(\sqrt{\eta}) \right) + 8 \left( \mathbf{H}_{0,0,1}(\sqrt{\eta}) + \mathbf{H}_{0,0,-1}(\sqrt{\eta}) \right) \right] - \frac{8}{27(1-z)}\zeta_2 - F_1^{D_2}(z) + F_+^{D_2}(z), \quad (7.124)$$

$$D_2^{A,\text{reg},\varepsilon^0}(z) \propto \frac{2\mathbf{H}_0(\eta)Q_1}{81\eta z} + \frac{2Q_4}{729\eta z^2} + \frac{10(3-2\eta)}{81\eta z^{5/2}} + \frac{(45-10\eta-54z-810\eta z)}{81\eta z^{5/2}} \left( \mathbf{H}_0(\eta) + \mathbf{H}_1 + 2\mathbf{H}_{-1}(\sqrt{z}) - 2\ln(2) \right) - \frac{Q_5}{108\eta^{3/2}\pi z^{5/2}\sqrt{1-z}} \left\{ \mathbf{H}_0^2(\eta) [\mathbf{H}_{-1}(\sqrt{\eta}) + \mathbf{H}_1(\sqrt{\eta})] - 4\mathbf{H}_0(\eta) [\mathbf{H}_{0,1}(\sqrt{\eta}) + \mathbf{H}_{0,-1}(\sqrt{\eta})] + 8 [\mathbf{H}_{0,0,1}(\sqrt{\eta}) + \mathbf{H}_{0,0,-1}(\sqrt{\eta})] \right\} - \frac{8(89-84z+28z^2)}{27z}\mathbf{H}_0^2(\eta) - \frac{32Q_6}{27z}\mathbf{H}_0^3(\eta) + \left[ \frac{2Q_2}{81\eta z} - \frac{16(37-36z+11z^2)}{27z}\mathbf{H}_0(\eta) - \frac{8Q_6}{3z}\mathbf{H}_0^2(\eta) \right] \mathbf{H}_0 - \left[ \frac{8(59-60z+22z^2)}{81z} + \frac{8Q_6}{9z}\mathbf{H}_0(\eta) \right] \mathbf{H}_0^2 - \frac{8Q_6}{81z}\mathbf{H}_0^3 + \frac{8Q_6}{9z}\mathbf{H}_0^2(\eta)\mathbf{H}_1(\eta) + \left[ \frac{2Q_3}{81\eta z} + \frac{16(-5+4z+2z^2)}{9z}\mathbf{H}_0(\eta) - \frac{8Q_6}{9z}\mathbf{H}_0^2(\eta) \right] \mathbf{H}_1 - \frac{16(-2+z)(-26+11z)}{81z}\mathbf{H}_0 + \frac{8Q_6}{27z}\mathbf{H}_0^2 \mathbf{H}_1 - \frac{16Q_6}{9z}\mathbf{H}_0(\eta)\mathbf{H}_{0,1}(\eta) - \left[ \frac{8(59-60z+40z^2)}{81z} + \frac{8Q_6}{9z}\mathbf{H}_0(\eta) + \frac{8Q_6}{27z}\mathbf{H}_0 \right] \mathbf{H}_1^2 + \left[ \frac{16(5-4z)}{9z} - \frac{16Q_6}{9z}\mathbf{H}_0(\eta) - \frac{16Q_6}{9z}\mathbf{H}_0 + \frac{16Q_6}{9z}\mathbf{H}_1 \right] \mathbf{H}_{0,1}$$

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$$\begin{aligned}
& + \frac{8Q_6}{81z} H_1^3 + \frac{16Q_6}{9z} H_{0,0,1}(\eta) + \frac{32Q_6}{9z} H_{0,0,1} - \frac{32Q_6}{9z} H_{0,1,1} \\
& - \left[ \frac{8(163 - 156z + 98z^2)}{81z} + \frac{8Q_6}{9z} H_0(\eta) + \frac{40Q_6}{27z} H_0 + \frac{8Q_6}{27z} H_1 \right] \zeta_2 \\
& - \frac{32Q_6}{27z} \zeta_3 + F_7^{D_2}(z) + \int_z^1 dy \left[ \frac{\sqrt{y}}{2z^{3/2}} F_2^{D_2}(y) + \frac{y^{3/2}}{2z^{5/2}} F_3^{D_2}(y) + \frac{1}{y} F_4^{D_2}(y) \right. \\
& \left. + \frac{z}{y^2} F_5^{D_2}(y) - \frac{1}{z} H_0 \left( \frac{z}{y} \right) F_6^{D_2}(y) - \frac{1}{z} F_6^{D_2}(y) - \left( 6 - \frac{6}{y} - 4z + \frac{4z}{y^2} \right) F_+^{D_2}(y) \right] \\
& - \left( 6 - \frac{5}{z} - 4z \right) \int_0^z dy F_+^{D_2}(y) , \tag{7.125}
\end{aligned}$$

with the polynomials

$$Q_1 = -1600\eta + 3(39\eta^2 + 710\eta + 15)z + 6(4\eta^2 - 221\eta - 3)z^2 , \tag{7.126}$$

$$Q_2 = -176\eta + 9(13\eta^2 + 66\eta + 5)z + 2(12\eta^2 - 199\eta - 9)z^2 , \tag{7.127}$$

$$Q_3 = 1248\eta + 3(39\eta^2 - 314\eta + 15)z + 2(12\eta^2 + 265\eta - 9)z^2 , \tag{7.128}$$

$$\begin{aligned}
Q_4 = & 45(2\eta - 9) + (351 - 17000\eta)z + 6(315\eta^2 + 2761\eta - 108)z^2 \\
& + 2(324\eta^2 - 6017\eta + 81)z^3 , \tag{7.129}
\end{aligned}$$

$$\begin{aligned}
Q_5 = & -10 + (270\eta + 23)z + (9\eta^3 + 783\eta^2 - 729\eta - 39)z^2 \\
& + (62\eta^3 - 810\eta^2 + 810\eta + 34)z^3 + 8(4\eta^3 + 27\eta^2 - 54\eta - 1)z^4 , \tag{7.130}
\end{aligned}$$

$$Q_6 = 5 - 6z + 4z^2 . \tag{7.131}$$

The functions  $F_k$  are given by

$$\begin{aligned}
F_1^{D_2}(z) = & -\frac{2zR_1}{27(1-z)} - \frac{2R_2}{27} - \frac{2(27-8\eta)}{27\sqrt{z}(1-z)^{3/2}} G_1(z) \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\} \\
& - \frac{5(1+\eta)(27-8\eta)}{81\pi\sqrt{z}(1-z)^{3/2}} - \frac{2(27-8\eta)(1+\eta+\eta^2)}{81(1-\eta)\pi\sqrt{z}(1-z)^{3/2}} H_0(\eta) \\
& - \frac{\eta(1+\eta)(27-8\eta)}{54(1-\eta)^2\pi\sqrt{z}(1-z)^{3/2}} H_0^2(\eta) - \frac{(27-8\eta)}{54\sqrt{z}(1-z)^{3/2}} \left\{ 4(1+\eta) \left[ G_6(z) + G_7(z) \right. \right. \\
& \left. \left. - \frac{8}{\pi} (K_{19} + K_{20}) \right] - (1-\eta)^2 \left[ G_{12}(z) + G_{13}(z) - K_{13} - K_{14} + H_0(\eta) \right. \right. \\
& \left. \left. \times \left( G_4(z) - K_6 \right) + \frac{8}{\pi} \left( K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15} \right) \right] \right\} \\
& + \frac{R_3}{27(1-z+\eta z)} [H_0(\eta) + H_0 + H_1] + \frac{(27-8\eta)}{36\pi\sqrt{z}(1-z)^{3/2}} \zeta_2 \\
& \times \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\} , \tag{7.132}
\end{aligned}$$

$$\begin{aligned}
F_2^{D_2}(y) = & \frac{4R_4}{3\eta^2} + \frac{4(1+15\eta)}{3\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\} + \frac{10(1+\eta)(1+15\eta)}{9\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
& + \frac{4(1+15\eta)(1+\eta+\eta^2)}{9(1-\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) + \frac{(1+\eta)(1+15\eta)}{3(1-\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} H_0^2(\eta) \\
& + \frac{1+15\eta}{3\eta^2\sqrt{1-y}\sqrt{y}} \left\{ 4(1+\eta) \left[ G_6(y) + G_7(y) - \frac{8}{\pi} (K_{19} + K_{20}) \right] - (1-\eta)^2 \right.
\end{aligned}$$

$$\begin{aligned}
 & \times \left[ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} + H_0(\eta) \left( G_4(y) - K_6 \right) + \frac{8}{\pi} \left( K_{21} + K_{22} + K_{23} \right. \right. \\
 & \left. \left. + K_{24} + H_0(\eta) K_{15} \right) \right] \left. \right\} - \frac{2R_5}{3\eta^2(1-y+\eta y)} [H_0(\eta) + H_0(y) + H_1(y)] \\
 & - \frac{1+15\eta}{2\eta^2\pi\sqrt{1-y\sqrt{y}}} \zeta_2 \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\}, \tag{7.133}
 \end{aligned}$$

$$\begin{aligned}
 F_3^{D_2}(y) &= \frac{10(\eta+y-\eta y)}{9\eta^2} - \frac{10}{9\eta^2\sqrt{1-y\sqrt{y}}} G_1(y) \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\} \\
 & - \frac{25(1+\eta)}{27\eta^2\pi\sqrt{1-y\sqrt{y}}} - \frac{10(1+\eta+\eta^2)}{27(1-\eta)\eta^2\pi\sqrt{1-y\sqrt{y}}} H_0(\eta) - \frac{5(1+\eta)}{18(1-\eta)^2\eta\pi\sqrt{1-y\sqrt{y}}} H_0^2(\eta) \\
 & + \frac{1}{18\eta^2\sqrt{1-y\sqrt{y}}} \left\{ -20(1+\eta) \left[ G_6(y) + G_7(y) - \frac{8}{\pi} \left( K_{19} + K_{20} \right) \right] + 5(1-\eta)^2 \right. \\
 & \times \left[ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} + H_0(\eta) \left( G_4(y) - K_6 \right) + \frac{8}{\pi} \left( K_{21} + K_{22} + K_{23} \right. \right. \\
 & \left. \left. + K_{24} + H_0(\eta) K_{15} \right) \right] \left. \right\} + \frac{5R_6}{27\eta^2(1-y+\eta y)} [H_0(\eta) + H_0(y) + H_1(y)] \\
 & + \frac{5}{12\eta^2\pi\sqrt{1-y\sqrt{y}}} \zeta_2 \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\}, \tag{7.134}
 \end{aligned}$$

$$\begin{aligned}
 F_4^{D_2}(y) &= -\frac{2R_7}{9\eta^2} - \frac{2(1-\eta)(5+104\eta-13\eta^2)}{9\eta^2\sqrt{1-y\sqrt{y}}} G_1(y) \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\} \\
 & - \frac{5(1-\eta^2)(5+104\eta-13\eta^2)}{27\eta^2\pi\sqrt{1-y\sqrt{y}}} - \frac{2(1+\eta+\eta^2)(5+104\eta-13\eta^2)}{27\eta^2\pi\sqrt{1-y\sqrt{y}}} H_0(\eta) \\
 & - \frac{(1+\eta)(-5-104\eta+13\eta^2)}{18(-1+\eta)\eta\pi\sqrt{1-y\sqrt{y}}} H_0^2(\eta) - \frac{(1-\eta)(5+104\eta-13\eta^2)}{18\eta^2\sqrt{1-y\sqrt{y}}} \left\{ 4(1+\eta) \right. \\
 & \times \left[ G_6(y) + G_7(y) - \frac{8}{\pi} \left( K_{19} + K_{20} \right) \right] - (1-\eta)^2 \left[ G_{12}(y) + G_{13}(y) - K_{13} \right. \\
 & \left. \left. - K_{14} + H_0(\eta) \left( G_4(y) - K_6 \right) + \frac{8}{\pi} \left( K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta) K_{15} \right) \right] \right\} \\
 & + \frac{R_9}{9\eta^2(1-y+\eta y)} H_0(\eta) - \frac{(1-\eta)R_8}{9\eta^2(1-y+\eta y)} [H_0(y) + H_1(y)] \\
 & + \frac{(1-\eta)(5+104\eta-13\eta^2)}{12\eta^2\pi\sqrt{1-y\sqrt{y}}} \zeta_2 \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\}, \tag{7.135}
 \end{aligned}$$

$$\begin{aligned}
 F_5^{D_2}(y) &= -\frac{4R_{10}}{9\eta^2} + \frac{4(1+54\eta-27\eta^2-4\eta^3)}{9\eta^2\sqrt{1-y\sqrt{y}}} G_1(y) \left\{ 2(1-\eta) + (1+\eta)H_0(\eta) \right\} \\
 & + \frac{10(1+\eta)(1+54\eta-27\eta^2-4\eta^3)}{27\eta^2\pi\sqrt{1-y\sqrt{y}}} + \frac{4(1+\eta+\eta^2)(1+54\eta-27\eta^2-4\eta^3)}{27(1-\eta)\eta^2\pi\sqrt{1-y\sqrt{y}}} H_0(\eta) \\
 & + \frac{(1+\eta)(1+54\eta-27\eta^2-4\eta^3)}{9(1-\eta)^2\eta\pi\sqrt{1-y\sqrt{y}}} H_0^2(\eta) + \frac{1+54\eta-27\eta^2-4\eta^3}{9\eta^2\sqrt{1-y\sqrt{y}}} \left\{ 4(1+\eta) \right. \\
 & \times \left[ G_6(y) + G_7(y) - \frac{8}{\pi} \left( K_{19} + K_{20} \right) \right] - (1-\eta)^2 \left[ G_{12}(y) + G_{13}(y) - K_{13} \right. \\
 & \left. \left. - K_{14} + H_0(\eta) \left( G_4(y) - K_6 \right) + \frac{8}{\pi} \left( K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta) K_{15} \right) \right] \right\}
 \end{aligned}$$

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$$\begin{aligned}
& + \frac{2R_{11}}{27\eta^2(1-y+\eta y)} [\mathbf{H}_0(\eta) + \mathbf{H}_0(y) + \mathbf{H}_1(y)] - \frac{1+54\eta-27\eta^2-4\eta^3}{6\eta^2\pi\sqrt{1-y}\sqrt{y}} \zeta_2 \\
& \times \left\{ 2(1-\eta) + (1+\eta)\mathbf{H}_0(\eta) \right\} , \tag{7.136}
\end{aligned}$$

$$F_6^{D_2}(y) = \frac{80(1-\eta)}{9-9(1-\eta)y} (\mathbf{H}_0(\eta) + \mathbf{H}_0(y) + \mathbf{H}_1(y)) , \tag{7.137}$$

$$\begin{aligned}
F_7^{D_2}(y) &= \frac{2R_{12}}{27\eta} - \frac{2(81-189\eta-103\eta^2)}{27\eta\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(1-\eta) + (1+\eta)\mathbf{H}_0(\eta) \right\} \\
& - \frac{5(1+\eta)(81-189\eta-103\eta^2)}{81\eta\pi\sqrt{1-y}\sqrt{y}} - \frac{2(1+\eta+\eta^2)(81-189\eta-103\eta^2)}{81(1-\eta)\eta\pi\sqrt{1-y}\sqrt{y}} \mathbf{H}_0(\eta) \\
& - \frac{(1+\eta)(81-189\eta-103\eta^2)}{54(1-\eta)^2\pi\sqrt{1-y}\sqrt{y}} \mathbf{H}_0^2(\eta) - \frac{(81-189\eta-103\eta^2)}{54\eta\sqrt{1-y}\sqrt{y}} \left\{ 4(1+\eta) \right. \\
& \times \left[ G_6(y) + G_7(y) - \frac{8}{\pi} (K_{19} + K_{20}) \right] - (1-\eta)^2 \left[ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
& \left. \left. + \mathbf{H}_0(\eta) \left( G_4(y) - K_6 \right) + \frac{8}{\pi} \left( K_{21} + K_{22} + K_{23} + K_{24} + \mathbf{H}_0(\eta)K_{15} \right) \right] \right\} \\
& + \frac{R_{13}}{27\eta(1-y+\eta y)} [\mathbf{H}_0(\eta) + \mathbf{H}_0(y) + \mathbf{H}_1(y)] + \frac{81-189\eta-103\eta^2}{36\eta\pi\sqrt{1-y}\sqrt{y}} \zeta_2 \\
& \times \left\{ 2(1-\eta) + (1+\eta)\mathbf{H}_0(\eta) \right\} , \tag{7.138}
\end{aligned}$$

$$F_+^{D_2}(z) = \frac{8}{9(1-z)} \left\{ 2(1-\eta) [G_{10}(z) + G_{11}(z)] + \mathbf{H}_0^2(\eta) + 2(1-\eta)\mathbf{H}_0(\eta)G_3(z) \right\} \tag{7.139}$$

The functions  $G_i$  and  $K_i$  are given in Appendix H.2. The additional polynomials read

$$R_1 = -(8\eta - 27) [\eta(1-z) - z] , \tag{7.140}$$

$$R_2 = (8\eta - 27) [\eta(1+z) + z] , \tag{7.141}$$

$$R_3 = (8\eta - 27) [2\eta + (\eta^2 - 1)z] , \tag{7.142}$$

$$R_4 = -(15\eta + 1) [(1-\eta)y + \eta] , \tag{7.143}$$

$$R_5 = (15\eta + 1) [-\eta^2 + (-\eta^2 + 2\eta + 1)y + (\eta^2 - 1)y^2] , \tag{7.144}$$

$$R_6 = \eta^2(2\eta - 5) + (-3\eta^2 + 6\eta + 3)y + 3(\eta^2 - 1)y^2 , \tag{7.145}$$

$$R_7 = -(13\eta^3 - 117\eta^2 + 99\eta + 5) [(1-\eta)y + \eta] , \tag{7.146}$$

$$R_8 = (13\eta^2 - 104\eta - 5) y (1 - \eta^2 + 2\eta + (\eta^2 - 1) y) , \tag{7.147}$$

$$R_9 = (13\eta^3 - 117\eta^2 + 99\eta + 5) y (1 - \eta^2 + 2\eta + (\eta^2 - 1) y) , \tag{7.148}$$

$$R_{10} = -(4\eta^3 + 27\eta^2 - 54\eta - 1) [(1-\eta)y + \eta] , \tag{7.149}$$

$$\begin{aligned}
R_{11} &= -2\eta^2 (4\eta^2 + 31\eta - 71) - 3 (4\eta^5 + 19\eta^4 - 112\eta^3 + 80\eta^2 + 56\eta + 1) y \\
& + 3 (4\eta^5 + 27\eta^4 - 58\eta^3 - 28\eta^2 + 54\eta + 1) y^2 , \tag{7.150}
\end{aligned}$$

$$R_{12} = -(103\eta^2 + 189\eta - 81) [(1-\eta)y + \eta] , \tag{7.151}$$

$$\begin{aligned}
R_{13} &= \eta (112\eta^2 + 152\eta - 53) + (103\eta^4 - 17\eta^3 - 562\eta^2 - 27\eta + 81) y \\
& + (-103\eta^4 - 189\eta^3 + 184\eta^2 + 189\eta - 81) y^2 . \tag{7.152}
\end{aligned}$$

The final result is defined on the usual support  $x \in [0, 1]$  although single sums with support other

than  $z \in [0, 1]$ , as for example

$$S_1 \left( \left\{ \frac{1}{1-\eta} \right\}, N \right) = \int_0^{1/(1-\eta)} dz \frac{z^N - 1}{z - 1}, \quad (7.153)$$

contribute. The contributions in other domains cancel analytically.

### 7.2.2. Fixed moments of $\tilde{A}_{gg,Q}^{(3)}$

In Ref. [202] the fixed moments  $N = 2, 4, 6$  of all two-mass OMEs at 3-loop order were presented as series expansions up to  $\mathcal{O}(\eta^3 L_\eta^2)$  using the programs Q2E and EXP [200, 201]. However, for the constant part of  $\hat{A}_{gg,Q}^{(3)}$  and  $\hat{A}_{Qg}^{(3)}$ , only the irreducible contributions were given. To allow for a direct comparison with the general  $N$  results presented later, we list the corresponding expressions including the reducible parts for  $\hat{A}_{gg,Q}^{(3)}$  in the following. They are given by

$$\begin{aligned} \tilde{a}_{gg,Q}^{(3)}(N=2) = & C_F T_F^2 \left\{ -\frac{25556}{729} + \left( -\frac{512}{9} + \frac{160}{9} L_1 + \frac{160}{9} L_2 \right) \zeta_2 - \frac{1408}{81} \zeta_3 - \frac{3484}{81} L_1 - \frac{1336}{27} L_1^2 + \frac{992}{81} L_1^3 \right. \\ & - \frac{16820}{243} L_2 - \frac{1936}{27} L_1 L_2 + \frac{64}{27} L_1^2 L_2 - \frac{1336}{27} L_2^2 + \frac{320}{27} L_1 L_2^2 + \frac{736}{81} L_2^3 + \eta \left( \frac{758944}{30375} + \frac{22976}{2025} L_\eta \right. \\ & \left. - \frac{448}{135} L_\eta^2 \right) + \eta^2 \left( -\frac{169892864}{10418625} + \frac{1028192}{99225} L_\eta - \frac{4768}{945} L_\eta^2 \right) + \eta^3 \left( -\frac{826805984}{843908625} + \frac{5893184}{2679075} L_\eta \right. \\ & \left. - \frac{23872}{8505} L_\eta^2 \right) \left. \right\} + C_A T_F^2 \left\{ -\frac{59314}{2187} + \left( \frac{1340}{81} - \frac{308}{9} L_1 - \frac{308}{9} L_2 \right) \zeta_2 + \frac{176}{81} \zeta_3 - \frac{6844}{243} L_1 \right. \\ & + \frac{1090}{81} L_1^2 - \frac{1276}{81} L_1^3 + 12 L_2 + \frac{1840}{81} L_1 L_2 - \frac{440}{27} L_1^2 L_2 + \frac{1090}{81} L_2^2 - \frac{616}{27} L_1 L_2^2 - \frac{1100}{81} L_2^3 \\ & + \eta \left( -\frac{256304}{10125} + \frac{7184}{675} L_\eta + \frac{8}{45} L_\eta^2 \right) + \eta^2 \left( -\frac{1565036}{496125} + \frac{6008}{4725} L_\eta + \frac{8}{45} L_\eta^2 \right) \\ & \left. + \eta^3 \left( -\frac{56086736}{843908625} - \frac{164464}{2679075} L_\eta + \frac{2552}{8505} L_\eta^2 \right) \right\} + T_F^3 \left\{ \left( 32 L_1 + 32 L_2 \right) \zeta_2 \right. \\ & \left. + \frac{128}{9} \zeta_3 + \frac{32}{3} L_1^3 + \frac{64}{3} L_1^2 L_2 + \frac{64}{3} L_1 L_2^2 + \frac{32}{3} L_2^3 \right\} + \mathcal{O}(\eta^4 L_\eta^3), \quad (7.154) \end{aligned}$$

$$\begin{aligned} \tilde{a}_{gg,Q}^{(3)}(N=4) = & C_F T_F^2 \left\{ -\frac{934723727}{21870000} + \left( -\frac{226583}{4050} + \frac{121}{45} L_1 + \frac{121}{45} L_2 \right) \zeta_2 - \frac{5324}{2025} \zeta_3 - \frac{9432079}{243000} L_1 \right. \\ & - \frac{2051797}{40500} L_1^2 + \frac{3751}{2025} L_1^3 - \frac{3415493}{81000} L_2 - \frac{673474}{10125} L_1 L_2 + \frac{242}{675} L_1^2 L_2 - \frac{2051797}{40500} L_2^2 \\ & + \frac{242}{135} L_1 L_2^2 + \frac{2783}{2025} L_2^3 + \eta \left( \frac{1556008}{253125} + \frac{18544}{5625} L_\eta - \frac{416}{1125} L_\eta^2 \right) + \eta^2 \left( -\frac{92973466}{17364375} + \frac{160036}{55125} L_\eta \right. \\ & \left. - \frac{428}{315} L_\eta^2 \right) + \eta^3 \left( -\frac{1109454088}{4219543125} + \frac{4900048}{13395375} L_\eta - \frac{35648}{42525} L_\eta^2 \right) \left. \right\} + C_A T_F^2 \left\{ -\frac{518340979}{1822500} \right. \\ & + \left( -\frac{32182}{675} - \frac{3304}{45} L_1 - \frac{3304}{45} L_2 \right) \zeta_2 + \frac{1888}{405} \zeta_3 - \frac{13735499}{60750} L_1 - \frac{31169}{675} L_1^2 - \frac{13688}{405} L_1^3 \\ & \left. - \frac{811661}{6750} L_2 - \frac{34208}{675} L_1 L_2 - \frac{944}{27} L_1^2 L_2 - \frac{31169}{675} L_2^2 - \frac{6608}{135} L_1 L_2^2 - \frac{2360}{81} L_2^3 \right\} \end{aligned}$$

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$$\begin{aligned}
& +\eta\left(-\frac{22204183}{303750} + \frac{697393}{20250}L_\eta - \frac{7303}{2700}L_\eta^2\right) + \eta^2\left(-\frac{94581301}{10418625} + \frac{492763}{99225}L_\eta - \frac{205}{189}L_\eta^2\right) \\
& +\eta^3\left(-\frac{692255687}{1687817250} + \frac{3118727}{5358150}L_\eta - \frac{7319}{34020}L_\eta^2\right)\} + T_F^3\left\{\left(32L_1 + 32L_2\right)\zeta_2 + \frac{128}{9}\zeta_3\right. \\
& \left. + \frac{32}{3}L_1^3 + \frac{64}{3}L_1^2L_2 + \frac{64}{3}L_1L_2^2 + \frac{32}{3}L_2^3\right\} + \mathcal{O}\left(\eta^4L_\eta^3\right), \tag{7.155}
\end{aligned}$$

$$\tilde{a}_{gg,Q}^{(3)}(N=6) =$$

$$\begin{aligned}
& C_A T_F^2 \left\{ -\frac{68860626799}{187535250} + \left( -\frac{193394}{2835} - \frac{806}{9}L_1 - \frac{806}{9}L_2 \right) \zeta_2 + \frac{3224}{567}\zeta_3 - \frac{9618442}{33075}L_1 \right. \\
& - \frac{1294861}{19845}L_1^2 - \frac{23374}{567}L_1^3 - \frac{1919194}{11907}L_2 - \frac{1471552}{19845}L_1L_2 - \frac{8060}{189}L_1^2L_2 - \frac{1294861}{19845}L_2^2 \\
& \left. - \frac{1612}{27}L_1L_2^2 - \frac{20150}{567}L_2^3 + \eta\left(-\frac{488831873}{5315625} + \frac{14655008}{354375}L_\eta - \frac{12167}{3375}L_\eta^2\right) \right. \\
& \left. + \eta^2\left(-\frac{469449112}{52093125} + \frac{2525176}{496125}L_\eta - \frac{232}{225}L_\eta^2\right) + \eta^3\left(-\frac{1795386647}{4219543125} + \frac{8701352}{13395375}L_\eta \right. \right. \\
& \left. \left. - \frac{4819}{42525}L_\eta^2\right)\right\} + C_F T_F^2 \left\{ -\frac{705306787007}{15315378750} + \left( -\frac{4410376}{77175} + \frac{484}{441}L_1 + \frac{484}{441}L_2 \right) \zeta_2 - \frac{21296}{19845}\zeta_3 \right. \\
& - \frac{2991682411}{72930375}L_1 - \frac{12017984}{231525}L_1^2 + \frac{15004}{19845}L_1^3 - \frac{334770739}{8103375}L_2 - \frac{15657416}{231525}L_1L_2 + \frac{968}{6615}L_1^2L_2 \\
& - \frac{12017984}{231525}L_2^2 + \frac{968}{1323}L_1L_2^2 + \frac{11132}{19845}L_2^3 + \eta\left(\frac{3661888}{826875} + \frac{10784}{3375}L_\eta - \frac{1216}{11025}L_\eta^2\right) \\
& \left. + \eta^2\left(-\frac{930064}{180075} + \frac{589024}{231525}L_\eta - \frac{1504}{1225}L_\eta^2\right) + \eta^3\left(-\frac{283956224}{1181472075} + \frac{2587744}{18753525}L_\eta - \frac{251008}{297675}L_\eta^2\right)\right\} \\
& + T_F^3 \left\{ \left(32L_1 + 32L_2\right)\zeta_2 + \frac{128}{9}\zeta_3 + \frac{32}{3}L_1^3 + \frac{64}{3}L_1^2L_2 + \frac{64}{3}L_1L_2^2 + \frac{32}{3}L_2^3 \right\} + \mathcal{O}\left(\eta^4L_\eta^3\right). \tag{7.156}
\end{aligned}$$

The expressions for  $\hat{A}_{Qg}^{(3)}$  will be given in Section 7.3.

### 7.2.3. The $N$ -space Solution

For the constant part of the OME  $\tilde{A}_{gg,Q}^{(3)}$  in Mellin  $N$ -space one obtains

$$\begin{aligned}
& \tilde{a}_{gg,Q}^{(3)}(N) = \\
& \frac{1}{2}(1 + (-1)^N) \left\{ T_F^3 \left\{ \frac{32}{3}(L_1^3 + L_2^3) + \frac{64}{3}L_1L_2(L_1 + L_2) + 32\zeta_2(L_1 + L_2) + \frac{128}{9}\zeta_3 \right\} \right. \\
& + C_F T_F^2 \left\{ \frac{(2 + N + N^2)^2}{(N-1)N^2(N+1)^2(N+2)} \left[ 24L_1^3 + 24L_2^3 + 16L_1L_2(L_1 + L_2) \right. \right. \\
& + 48H_0(\eta)(L_1^2 - L_2^2) + 16(L_1^2 + L_2^2)S_1 + 32S_1H_0(\eta)(L_1 - L_2) + \left( 48H_0^2(\eta) + \frac{16}{3}S_1^2 \right. \\
& \left. \left. - 16S_2 + 40\zeta_2 \right) (L_1 + L_2) - \frac{32}{9}H_0^3(\eta) - \frac{64}{3}H_0^2(\eta)H_1(\eta) + \frac{128}{3}H_0(\eta)H_{0,1}(\eta) - \frac{352}{9}\zeta_3 \right. \\
& \left. - \frac{128}{3}H_{0,0,1}(\eta) + 32\left(H_0^2(\eta) - \frac{1}{3}S_2\right)S_1 + \frac{32}{27}S_1^3 - \frac{704}{27}S_3 + \frac{128}{3}S_{2,1} + \frac{32}{3}\zeta_2S_1 \right. \\
& \left. \left. - \frac{32}{3}H_0^2(\eta)\left(S_1\left(\frac{1}{1-\eta}, N\right) + S_1\left(\frac{\eta}{\eta-1}, N\right)\right) + \frac{64}{3}S_{1,2}\left(\frac{1}{1-\eta}, 1-\eta, N\right) \right\} \right.
\end{aligned}$$



$$\begin{aligned}
 & -\frac{64}{3}H_0(\eta)\left(S_{1,1}\left(\frac{1}{1-\eta}, 1-\eta, N\right) - S_{1,1}\left(\frac{\eta}{\eta-1}, \frac{\eta-1}{\eta}, N\right)\right) \\
 & -\frac{64}{3}S_{1,1,1}\left(\frac{1}{1-\eta}, 1-\eta, 1, N\right) - \frac{64}{3}S_{1,1,1}\left(\frac{\eta}{\eta-1}, \frac{\eta-1}{\eta}, 1, N\right) \\
 & +\frac{64}{3}S_{1,2}\left(\frac{\eta}{\eta-1}, \frac{\eta-1}{\eta}, N\right)\left] + \frac{P_{167}L_1 + P_{168}L_2}{54\eta(N-1)N^4(N+1)^4(N+2)} \right. \\
 & -\frac{(1+\eta)(5-2\eta+5\eta^2)}{4\eta^{3/2}}\left[\frac{1}{4}\left(H_1(\sqrt{\eta}) + H_{-1}(\sqrt{\eta})\right)(L_1 - L_2)^2 \right. \\
 & + \left.(H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}))\left(L_1 - L_2\right) + 2H_{0,0,1}(\sqrt{\eta}) + 2H_{0,0,-1}(\sqrt{\eta})\right] \\
 & +\frac{1}{(N-1)N^3(N+1)^3(N+2)}\left[\frac{P_{154}}{24\eta}\left(L_1^2 + L_2^2\right) + \frac{P_{153}}{12\eta}L_1L_2 + \frac{32}{9}P_{133}\left(L_1 + L_2\right)S_1 \right. \\
 & +\left.\frac{32}{3}P_{133}H_0(\eta)\left(L_1 - L_2\right) + \frac{32}{27}P_{133}S_1^2 - \frac{32}{9}P_{133}S_2 + \frac{32}{3}P_{133}H_0^2(\eta) - \frac{16}{9}\zeta_2P_{149}\right] \\
 & -\frac{16P_{166}}{81\eta(N-1)N^4(N+1)^4(N+2)(2N-3)(2N-1)}S_1 \\
 & +\frac{16P_{126}}{3\eta(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)}H_0(\eta) \\
 & +\frac{P_{171}}{243\eta(N-1)N^5(N+1)^5(N+2)(2N-3)(2N-1)} \\
 & -\frac{4P_{146}(1-\eta)^{-N}}{3\eta(N-1)N^3(N+1)^2(N+2)(2N-3)(2N-1)}\left[H_0^2(\eta) \right. \\
 & +\left.2H_0(\eta)S_1(1-\eta, N) - 2S_2(1-\eta, N) + 2S_{1,1}(1-\eta, 1, N)\right] \\
 & -\frac{4P_{145}}{3(N-1)N^3(N+1)^2(N+2)(2N-3)(2N-1)}\left(\frac{\eta}{1-\eta}\right)^N\left[H_0^2(\eta) \right. \\
 & -\left.2H_0(\eta)S_1\left(\frac{\eta-1}{\eta}, N\right) - 2S_2\left(\frac{\eta-1}{\eta}, N\right) + 2S_{1,1}\left(\frac{\eta-1}{\eta}, 1, N\right)\right] \\
 & -\frac{2(1+\eta)P_{138}2^{-2N}}{3\eta^{3/2}(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)}\binom{2N}{N}\left[H_0^2(\eta)\left(H_{-1}(\sqrt{\eta}) \right. \right. \\
 & +\left. H_1(\sqrt{\eta})\right) - 4H_0(\eta)\left(H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta})\right) + 8\left(H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta})\right)\left.\right] \\
 & -\frac{2^{2-2N}P_{132}}{3\eta(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)}\binom{2N}{N}\sum_{i=1}^N\frac{4^i\left(\frac{\eta}{\eta-1}\right)^i}{i^{\binom{2i}{i}}}\left[\frac{1}{2}H_0(\eta)^2 \right. \\
 & -\left. H_0(\eta)S_1\left(\frac{\eta-1}{\eta}, i\right) - S_2\left(\frac{\eta-1}{\eta}, i\right) + S_{1,1}\left(\frac{\eta-1}{\eta}, 1, i\right)\right] \\
 & +\frac{2^{3-2N}P_{140}}{3\eta(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)}\binom{2N}{N}\sum_{i=1}^N\frac{4^i}{i^2\binom{2i}{i}}\left(\frac{1}{i} - S_1(i)\right) \\
 & +\frac{(1-\eta^2)2^{4-2N}P_{134}}{3\eta(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)}\binom{2N}{N}H_0(\eta)\sum_{i=1}^N\frac{4^i}{i^2\binom{2i}{i}} \\
 & +\frac{2^{2-2N}P_{142}}{3\eta(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)}\binom{2N}{N}\sum_{i=1}^N\frac{4^i(1-\eta)^{-i}}{i^{\binom{2i}{i}}}\left[\frac{1}{2}H_0(\eta)^2 \right.
 \end{aligned}$$

$$\begin{aligned}
 & \left. + H_0(\eta)S_1(1 - \eta, i) - S_2(1 - \eta, i) + S_{1,1}(1 - \eta, 1, i) \right\} \\
 & + C_{AT_F}^2 \left\{ \frac{1}{(N-1)N(N+1)(N+2)} \left[ \frac{16}{9}P_{121}L_1^3 + \frac{8}{9}P_{124}L_2^3 - \frac{8}{3}P_{119}L_1^2L_2 - \frac{16}{3}P_{120}L_1L_2^2 \right] \right. \\
 & - \frac{16}{3}(5L_1^3 + 5L_2^3 + 2L_1^2L_2 + 2L_1L_2^2)S_1 + \frac{1}{(N-1)N^2(N+1)^2(N+2)} \left[ \frac{P_{143}}{54\eta}(L_1^2 + L_2^2) \right. \\
 & - \left. \frac{8}{27}P_{136}(L_1 + L_2)S_1 + \frac{P_{139}}{27\eta}L_1L_2 \right] + (L_1^2 + L_2^2) \left[ \frac{8}{3}H_1(\eta) + \frac{16(6 + 85N - 85N^2)}{27(N-1)N}S_1 \right] \\
 & + \frac{(1 + \eta)(4 + 11\eta + 4\eta^2)}{6\eta^{3/2}} \left[ -\frac{1}{2}(H_1(\sqrt{\eta}) + H_{-1}(\sqrt{\eta}))(L_1 - L_2)^2 \right. \\
 & - \left. 2(H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}))(L_1 - L_2) \right] - L_1L_2 \left[ \frac{64(3 - 10N + 10N^2)}{27(N-1)N}S_1 \right. \\
 & + \left. \frac{16}{3}H_1(\eta) \right] + (L_1^2 - L_2^2) \left[ \frac{2(1 + 2N)P_{123}}{(N-1)N(N+1)^2(N+2)}H_0(\eta) - 32H_0(\eta)S_1 \right] \\
 & + (L_1 + L_2) \left[ \frac{2P_{130}}{3(N-1)N(N+1)^2(N+2)}H_0^2(\eta) + \left( \frac{224(1 + N + N^2)}{3(N-1)N(N+1)(N+2)} \right. \right. \\
 & - \left. \left. \frac{112}{3}S_1 \right) \zeta_2 - \frac{64}{3}H_0^2(\eta)S_1 \right] + (L_1 - L_2) \left[ \frac{4P_{164}}{9(N-1)^2N^2(N+1)^3(N+2)^2}H_0(\eta) \right. \\
 & + \left. \frac{16}{3}H_{0,1}(\eta) - \frac{4P_{125}}{9(N-1)N(N+1)^2}H_0(\eta)S_1 - \frac{16}{3}H_0(\eta)S_1^2 - 16H_0(\eta)S_2 \right] \\
 & - \frac{2}{27\eta(N-1)N^3(N+1)^3(N+2)}(P_{155}L_1 - P_{156}L_2) \\
 & + \frac{2P_{170}}{3645\eta(N-1)N^4(N+1)^4(N+2)(2N-3)(2N-1)} \\
 & + \frac{1}{45\eta(N-1)N^2(N+1)^2(N+2)(2N-3)(2N-1)} \left[ P_{157}(1 - \eta)^{-N}S_2(1 - \eta, N) \right. \\
 & + P_{152}(1 - \eta)^{-N} \left( \frac{1}{2}H_0^2(\eta) + H_0(\eta)S_1(1 - \eta, N) + S_{1,1}(1 - \eta, 1, N) \right) \\
 & + \left( \frac{\eta}{1 - \eta} \right)^N \left\{ P_{148} \left[ \frac{1}{2}H_0^2(\eta) + S_{1,1} \left( \frac{\eta - 1}{\eta}, 1, N \right) \right] + P_{150} \left[ H_0(\eta)S_1 \left( \frac{\eta - 1}{\eta}, N \right) \right. \right. \\
 & + \left. \left. S_2 \left( \frac{\eta - 1}{\eta}, N \right) \right] \right\} + \left( \frac{(1 + \eta)2^{-2N}P_{158}}{90\eta^{3/2}(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)} \left( \frac{2N}{N} \right) \right. \\
 & - \left. \frac{(1 + \eta)(5 + 22\eta + 5\eta^2)}{9\eta^{3/2}}S_1 \right) \left[ H_0^2(\eta)(H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) \right. \\
 & - \left. 4H_0(\eta)(H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta})) + 8(H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta})) \right] \\
 & + \frac{P_{144}}{45\eta(N-1)N(N+1)(N+2)(2N-3)(2N-1)}H_0(\eta) \\
 & + \left[ \frac{P_{165}}{540\eta(N-1)^2N^2(N+1)^3(N+2)^2} - \frac{(1 + \eta)P_{128}H_{-1}(\sqrt{\eta})}{360\eta^{3/2}(N-1)N(N+1)(N+2)} \right] H_0^2(\eta) \\
 & - \frac{4P_{122}}{27(N-1)N(N+1)(N+2)}H_0(\eta) \left[ H_0(\eta)^2 + 6H_0(\eta)H_1(\eta) - 12H_{0,1}(\eta) \right]
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{(1+\eta)P_{128}}{360\eta^{3/2}(N-1)N(N+1)(N+2)}\mathbf{H}_0(\eta)\left[\mathbf{H}_0(\eta)\mathbf{H}_1(\sqrt{\eta})-4\mathbf{H}_{0,1}(\sqrt{\eta})-4\mathbf{H}_{0,-1}(\sqrt{\eta})\right] \\
 & -\frac{256(1+N+N^2)}{9(N-1)N(N+1)(N+2)}\mathbf{H}_{0,0,1}(\eta)-\frac{(1+\eta)P_{129}}{45\eta^{3/2}(N-1)N(N+1)(N+2)}\left(\mathbf{H}_{0,0,1}(\sqrt{\eta})\right. \\
 & \left.+\mathbf{H}_{0,0,-1}(\sqrt{\eta})\right)+\left[\frac{8P_{169}}{3645\eta(N-1)N^3(N+1)^3(N+2)(2N-3)(2N-1)}\right. \\
 & \left.+\frac{8P_{141}\mathbf{H}_0(\eta)}{45\eta(N-1)N^2(N+1)^2(N+2)}+\frac{2P_{127}\mathbf{H}_0^2(\eta)}{9\eta(N-1)N(N+1)^2}+\frac{32}{27}\mathbf{H}_0^3(\eta)+\frac{128}{9}\mathbf{H}_{0,0,1}(\eta)\right. \\
 & \left.+\frac{64}{9}\mathbf{H}_0^2(\eta)\mathbf{H}_1(\eta)-\frac{128}{9}\mathbf{H}_0(\eta)\mathbf{H}_{0,1}(\eta)\right]S_1-\frac{16P_{118}}{15\eta(N-1)N(N+1)}(S_3-S_{2,1}) \\
 & +\left[\frac{4P_{131}}{135\eta(N-1)N^2(N+1)^2(N+2)}-\frac{16}{3}\mathbf{H}_0^2(\eta)\right]S_1^2 \\
 & -\left[\frac{4P_{137}}{135\eta(N-1)N^2(N+1)^2(N+2)}-\frac{16P_{117}}{15\eta(N-1)N(N+1)}\mathbf{H}_0(\eta)+16\mathbf{H}_0^2(\eta)\right]S_2 \\
 & -\frac{16(1-7N+4N^2+4N^3)}{15\eta(N-1)N(N+1)}\left[\frac{1}{2}\mathbf{H}_0^2(\eta)\left(\eta^2S_1\left(\frac{1}{1-\eta},N\right)+S_1\left(\frac{\eta}{\eta-1},N\right)\right)\right. \\
 & \left.+\mathbf{H}_0(\eta)\left(\eta^2S_{1,1}\left(\frac{1}{1-\eta},1-\eta,N\right)-S_{1,1}\left(\frac{\eta}{\eta-1},\frac{\eta-1}{\eta},N\right)\right)\right. \\
 & \left.-S_{1,2}\left(\frac{\eta}{\eta-1},\frac{\eta-1}{\eta},N\right)+S_{1,1,1}\left(\frac{\eta}{\eta-1},\frac{\eta-1}{\eta},1,N\right)\right. \\
 & \left.-\eta^2S_{1,2}\left(\frac{1}{1-\eta},1-\eta,N\right)+\eta^2S_{1,1,1}\left(\frac{1}{1-\eta},1-\eta,1,N\right)\right] \\
 & +\frac{2^{-1-2N}}{45\eta^2(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)}\binom{2N}{N}\left[P_{147}\sum_{i=1}^N\frac{4^i\left(\frac{\eta}{\eta-1}\right)^i}{i\binom{2i}{i}}\left\{S_2\left(\frac{\eta-1}{\eta},i\right)+\mathbf{H}_0(\eta)S_1\left(\frac{\eta-1}{\eta},i\right)\right\}+P_{151}\sum_{i=1}^N\frac{4^i\left(\frac{\eta}{\eta-1}\right)^i}{i\binom{2i}{i}}\left\{S_{1,1}\left(\frac{\eta-1}{\eta},1,i\right)+\frac{1}{2}\mathbf{H}_0^2(\eta)\right\}+\eta P_{161}\sum_{i=1}^N\frac{4^i(1-\eta)^{-i}}{i\binom{2i}{i}}\left\{\frac{1}{2}\mathbf{H}_0^2(\eta)+\mathbf{H}_0(\eta)S_1(1-\eta,i)+S_{1,1}(1-\eta,1,i)\right\}+(1-\eta^2)P_{159}\mathbf{H}_0(\eta)\sum_{i=1}^N\frac{4^i}{i^2\binom{2i}{i}}+\eta P_{160}\sum_{i=1}^N\frac{4^i(1-\eta)^{-i}}{i\binom{2i}{i}}S_2(1-\eta,i)+P_{163}\sum_{i=1}^N\frac{4^i}{i^3\binom{2i}{i}}+P_{162}\sum_{i=1}^N\frac{4^i}{i^2\binom{2i}{i}}S_1(i)\right]+\left[\frac{8P_{135}}{27(N-1)N^2(N+1)^2(N+2)}-\frac{1120}{27}S_1\right]\zeta_2+\left[-\frac{128(1+N+N^2)}{27(N-1)N(N+1)(N+2)}+\frac{64}{27}S_1\right]\zeta_3\left.\right\}. \tag{7.157}
 \end{aligned}$$

The polynomials  $P_i$  read

$$P_{117} = (\eta^2 - 1)(4N^3 + 4N^2 - 7N + 1), \tag{7.158}$$

$$P_{118} = (\eta^2 + 1)(4N^3 + 4N^2 - 7N + 1), \tag{7.159}$$

$$P_{119} = N^4 + 2N^3 - 11N^2 - 16N - 12, \tag{7.160}$$

$$P_{120} = N^4 + 2N^3 - 6N^2 - 9N - 6, \tag{7.161}$$

$$P_{121} = 2N^4 + 4N^3 + 25N^2 + 17N + 24, \tag{7.162}$$

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$$\begin{aligned}
P_{122} &= 3N^4 + 6N^3 + 13N^2 + 10N + 16 , & (7.163) \\
P_{123} &= 3N^4 + 9N^3 + 15N^2 + 7N + 10 , & (7.164) \\
P_{124} &= 5N^4 + 10N^3 + 49N^2 + 32N + 48 , & (7.165) \\
P_{125} &= 92N^4 + 65N^3 - 152N^2 - 179N - 90 , & (7.166) \\
P_{126} &= (\eta^2 - 1) (5N^4 + 10N^3 + 73N^2 + 32N + 32) , & (7.167) \\
P_{127} &= (5\eta^2 - 102\eta + 5) N^4 + (5\eta^2 - 48\eta + 5) N^3 - (5\eta^2 - 206\eta + 5) N^2 \\
&\quad - (5\eta^2 - 244\eta + 5) N + 164\eta , & (7.168) \\
P_{128} &= 3 (71\eta^2 - 46\eta + 71) N^4 + 42 (17\eta^2 - 2\eta + 17) N^3 - (253\eta^2 + 1382\eta + 253) N^2 \\
&\quad - 2 (593\eta^2 + 862\eta + 593) N - 128 (2\eta^2 + 13\eta + 2) , & (7.169) \\
P_{129} &= 3 (111\eta^2 + 64\eta + 111) N^4 + 18 (53\eta^2 + 32\eta + 53) N^3 - (373\eta^2 + 1712\eta + 373) N^2 \\
&\quad - 2 (713\eta^2 + 1192\eta + 713) N - 128 (2\eta^2 + 13\eta + 2) , & (7.170) \\
P_{130} &= 12N^5 + 45N^4 + 87N^3 + 73N^2 + 69N + 14 , & (7.171) \\
P_{131} &= -140\eta N^5 - 190\eta N^4 + (63\eta^2 + 320\eta + 63) N^3 + 2 (108\eta^2 + 535\eta + 108) N^2 \\
&\quad + (279\eta^2 + 700\eta + 279) N - 2 (9\eta^2 - 160\eta + 9) , & (7.172) \\
P_{132} &= -36N^6 - 36\eta N^5 + (5\eta^2 - 18\eta + 225) N^4 + 2 (5\eta^2 - 108\eta + 9) N^3 \\
&\quad + (73\eta^2 + 246\eta - 495) N^2 + 8 (4\eta^2 + 21\eta + 27) N + 32\eta(\eta + 9) , & (7.173) \\
P_{133} &= 4N^6 + 3N^5 - 50N^4 - 129N^3 - 100N^2 - 56N - 24 , & (7.174) \\
P_{134} &= 9N^6 - 55N^4 - 2N^3 + 142N^2 - 46N + 8 , & (7.175) \\
P_{135} &= 99N^6 + 297N^5 + 631N^4 + 767N^3 + 1118N^2 + 784N + 168 , & (7.176) \\
P_{136} &= 344N^6 + 978N^5 + 209N^4 - 1032N^3 - 817N^2 - 210N - 96 , & (7.177) \\
P_{137} &= -440\eta N^6 - 1100\eta N^5 + 270\eta N^4 + (63\eta^2 + 1640\eta + 63) N^3 \\
&\quad + (216\eta^2 + 2810\eta + 216) N^2 + 3 (93\eta^2 + 700\eta + 93) N - 6 (3\eta^2 - 160\eta + 3) , & (7.178) \\
P_{138} &= -36\eta N^6 - 36\eta N^5 + (5\eta^2 + 202\eta + 5) N^4 + 2 (5\eta^2 - 104\eta + 5) N^3 \\
&\quad + (73\eta^2 - 322\eta + 73) N^2 + 32 (\eta^2 + 11\eta + 1) N + 32 (\eta^2 + 8\eta + 1) , & (7.179) \\
P_{139} &= -9 (4\eta^2 - 93\eta + 4) N^6 - 27 (4\eta^2 - 93\eta + 4) N^5 + (-36\eta^2 + 3589\eta - 36) N^4 \\
&\quad + 3 (36\eta^2 + 1211\eta + 36) N^3 + (72\eta^2 + 5942\eta + 72) N^2 + 4224\eta N + 768\eta , & (7.180) \\
P_{140} &= 18 (\eta^2 + 1) N^6 + 36\eta N^5 + (-115\eta^2 + 18\eta - 115) N^4 - 2 (7\eta^2 - 108\eta + 7) N^3 \\
&\quad + (211\eta^2 - 246\eta + 211) N^2 - 4 (31\eta^2 + 42\eta + 31) N - 16 (\eta^2 + 18\eta + 1) , & (7.181) \\
P_{141} &= (\eta^2 - 1) (25N^6 + 75N^5 + 25N^4 - 96N^3 - 122N^2 - 93N + 6) , & (7.182) \\
P_{142} &= 36\eta^2 N^6 + 36\eta N^5 + (-225\eta^2 + 18\eta - 5) N^4 - 2 (9\eta^2 - 108\eta + 5) N^3 \\
&\quad + (495\eta^2 - 246\eta - 73) N^2 - 8 (27\eta^2 + 21\eta + 4) N - 32(9\eta + 1) , & (7.183) \\
P_{143} &= 9 (4\eta^2 + 171\eta + 4) N^6 + 27 (4\eta^2 + 171\eta + 4) N^5 + (36\eta^2 + 11555\eta + 36) N^4 \\
&\quad - 3 (36\eta^2 - 4925\eta + 36) N^3 + (-72\eta^2 + 20890\eta - 72) N^2 + 14592\eta N + 3264\eta , & (7.184) \\
P_{144} &= (\eta^2 - 1) (52N^6 + 200N^5 - 1925N^4 + 2394N^3 - 1447N^2 + 622N - 3384) , & (7.185) \\
P_{145} &= 18N^7 - (5\eta + 9)N^6 - 2(5\eta + 48)N^5 + (111 - 73\eta)N^4 - 8(4\eta - 33)N^3 \\
&\quad - 8(4\eta + 21)N^2 - 96 , & (7.186) \\
P_{146} &= 18\eta N^7 - (9\eta + 5)N^6 - 2(48\eta + 5)N^5 + (111\eta - 73)N^4 \\
&\quad + 8(33\eta - 4)N^3 - 8(21\eta + 4)N^2 - 96\eta , & (7.187) \\
P_{147} &= -800N^8 - 8(270\eta + 269)N^7 + 4 (30\eta^2 - 1185\eta + 589) N^6 \\
&\quad - 6 (2\eta^3 + 55\eta^2 - 1440\eta - 1409) N^5 + (147\eta^3 - 1005\eta^2 + 945\eta - 3703) N^4 \\
&\quad + (471\eta^3 + 6075\eta^2 - 915\eta - 7383) N^3 + (-1599\eta^3 - 1095\eta^2 + 10815\eta + 3839) N^2
\end{aligned}$$

$$\begin{aligned}
 & + (-3117\eta^3 - 6015\eta^2 + 2085\eta + 1351) N - 6(91\eta^3 + 465\eta^2 + 645\eta + 127) , \quad (7.188) \\
 P_{148} = & -400N^8 - 4(128\eta + 219)N^7 - 4(3\eta^2 + 300\eta - 404) N^6 \\
 & + (-525\eta^2 + 2410\eta + 3419) N^5 - (489\eta^2 + 2750\eta + 3561) N^4 \\
 & - 3(157\eta^2 - 1958\eta + 637) N^3 + (1299\eta^2 + 4686\eta + 2875) N^2 \\
 & - 2(1581\eta^2 + 638\eta + 381) N + 48\eta(3\eta - 80) , \quad (7.189) \\
 P_{149} = & 33N^8 + 132N^7 + 106N^6 - 108N^5 - 74N^4 + 282N^3 + 245N^2 + 148N + 84 , \quad (7.190) \\
 P_{150} = & 400N^8 + (512\eta + 876)N^7 + 4(3\eta^2 + 300\eta - 404) N^6 \\
 & + (525\eta^2 - 2410\eta - 3419) N^5 + (489\eta^2 + 2750\eta + 3561) N^4 \\
 & + 3(157\eta^2 - 1958\eta + 637) N^3 - (1299\eta^2 + 4686\eta + 2875) N^2 \\
 & + 2(1581\eta^2 + 638\eta + 381) N + 48(80 - 3\eta)\eta , \quad (7.191) \\
 P_{151} = & 800N^8 + 8(270\eta + 269)N^7 - 4(30\eta^2 - 1185\eta + 589) N^6 \\
 & + 6(2\eta^3 + 55\eta^2 - 1440\eta - 1409) N^5 + (-147\eta^3 + 1005\eta^2 - 945\eta + 3703) N^4 \\
 & + (-471\eta^3 - 6075\eta^2 + 915\eta + 7383) N^3 + (1599\eta^3 + 1095\eta^2 - 10815\eta - 3839) N^2 \\
 & + (3117\eta^3 + 6015\eta^2 - 2085\eta - 1351) N + 6(91\eta^3 + 465\eta^2 + 645\eta + 127) , \quad (7.192) \\
 P_{152} = & -400\eta^2 N^8 - 4\eta(219\eta + 128)N^7 + 4(404\eta^2 - 300\eta - 3) N^6 \\
 & + (3419\eta^2 + 2410\eta - 525) N^5 - (3561\eta^2 + 2750\eta + 489) N^4 \\
 & - 3(637\eta^2 - 1958\eta + 157) N^3 + (2875\eta^2 + 4686\eta + 1299) N^2 \\
 & - 2(381\eta^2 + 638\eta + 1581) N + 48(3 - 80\eta) , \quad (7.193) \\
 P_{153} = & -3(5\eta^2 + 282\eta + 5) N^8 - 12(5\eta^2 + 282\eta + 5) N^7 - 4(15\eta^2 + 718\eta + 15) N^6 \\
 & + (30\eta^2 + 2716\eta + 30) N^5 + (75\eta^2 + 4486\eta + 75) N^4 \\
 & + (30\eta^2 - 868\eta + 30) N^3 - 1280\eta N^2 - 1024\eta N - 1024\eta , \quad (7.194) \\
 P_{154} = & 3(5\eta^2 - 422\eta + 5) N^8 + 12(5\eta^2 - 422\eta + 5) N^7 + 12(5\eta^2 - 326\eta + 5) N^6 \\
 & + (-30\eta^2 + 4196\eta - 30) N^5 - 25(3\eta^2 - 10\eta + 3) N^4 \\
 & - 10(3\eta^2 + 1718\eta + 3) N^3 - 14400\eta N^2 - 8448\eta N - 4352\eta , \quad (7.195) \\
 P_{155} = & (36\eta^2 - 93\eta - 36) N^8 + 12(12\eta^2 - 31\eta - 12) N^7 + 16(9\eta^2 - 376\eta - 9) N^6 \\
 & - 6(12\eta^2 + 2719\eta - 12) N^5 + (-180\eta^2 - 23011\eta + 180) N^4 \\
 & - 6(12\eta^2 + 3019\eta - 12) N^3 - 6032\eta N^2 + 1376\eta N + 1056\eta , \quad (7.196) \\
 P_{156} = & (36\eta^2 + 93\eta - 36) N^8 + 12(12\eta^2 + 31\eta - 12) N^7 + 16(9\eta^2 + 376\eta - 9) N^6 \\
 & + (-72\eta^2 + 16314\eta + 72) N^5 + (-180\eta^2 + 23011\eta + 180) N^4 \\
 & + (-72\eta^2 + 18114\eta + 72) N^3 + 6032\eta N^2 - 1376\eta N - 1056\eta , \quad (7.197) \\
 P_{157} = & 400\eta^2 N^8 + 4\eta(219\eta + 128)N^7 - 4(404\eta^2 - 300\eta - 3) N^6 \\
 & + (-3419\eta^2 - 2410\eta + 525) N^5 + (3561\eta^2 + 2750\eta + 489) N^4 \\
 & + 3(637\eta^2 - 1958\eta + 157) N^3 - (2875\eta^2 + 4686\eta + 1299) N^2 \\
 & + 2(381\eta^2 + 638\eta + 1581) N + 48(80\eta - 3) , \quad (7.198) \\
 P_{158} = & 400(\eta^2 - \eta + 1) N^8 + 4(269\eta^2 + \eta + 269) N^7 - 2(589\eta^2 - 1744\eta + 589) N^6 \\
 & + (-4221\eta^2 + 66\eta - 4221) N^5 + 2(889\eta^2 - 874\eta + 889) N^4 \\
 & + 12(288\eta^2 - 503\eta + 288) N^3 - 20(56\eta^2 + 187\eta + 56) N^2 \\
 & + (883\eta^2 + 1082\eta + 883) N + 654\eta^2 + 2676\eta + 654 , \quad (7.199) \\
 P_{159} = & 800(\eta^2 + 1) N^8 + 8(269\eta^2 + 270\eta + 269) N^7 - 4(589\eta^2 - 1185\eta + 589) N^6 \\
 & - 6(1409\eta^2 + 1442\eta + 1409) N^5 + 7(529\eta^2 - 114\eta + 529) N^4 \\
 & + 3(2461\eta^2 + 462\eta + 2461) N^3 - (3839\eta^2 + 12414\eta + 3839) N^2
 \end{aligned}$$

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$$- (1351\eta^2 + 5202\eta + 1351) N + 762\eta^2 + 3324\eta + 762 , \quad (7.200)$$

$$\begin{aligned} P_{160} = & -800\eta^3 N^8 - 8\eta^2(269\eta + 270)N^7 + 4\eta(589\eta^2 - 1185\eta + 30) N^6 \\ & + 6(1409\eta^3 + 1440\eta^2 - 55\eta - 2) N^5 + (-3703\eta^3 + 945\eta^2 - 1005\eta + 147) N^4 \\ & + (-7383\eta^3 - 915\eta^2 + 6075\eta + 471) N^3 + (3839\eta^3 + 10815\eta^2 - 1095\eta - 1599) N^2 \\ & + (1351\eta^3 + 2085\eta^2 - 6015\eta - 3117) N - 6(127\eta^3 + 645\eta^2 + 465\eta + 91) , \quad (7.201) \end{aligned}$$

$$\begin{aligned} P_{161} = & 800\eta^3 N^8 + 8\eta^2(269\eta + 270)N^7 - 4\eta(589\eta^2 - 1185\eta + 30) N^6 \\ & - 6(1409\eta^3 + 1440\eta^2 - 55\eta - 2) N^5 + (3703\eta^3 - 945\eta^2 + 1005\eta - 147) N^4 \\ & + (7383\eta^3 + 915\eta^2 - 6075\eta - 471) N^3 + (-3839\eta^3 - 10815\eta^2 + 1095\eta + 1599) N^2 \\ & + (-1351\eta^3 - 2085\eta^2 + 6015\eta + 3117) N + 6(127\eta^3 + 645\eta^2 + 465\eta + 91) , \quad (7.202) \end{aligned}$$

$$\begin{aligned} P_{162} = & -800(\eta^4 + 1) N^8 - 8(269\eta^4 + 270\eta^3 + 270\eta + 269) N^7 + 4(589\eta^4 - 1185 \\ & \eta^3 + 60\eta^2 - 1185\eta + 589) N^6 + (8454\eta^4 + 8628\eta^3 - 660\eta^2 + 8628\eta + 8454) N^5 \\ & + (-3703\eta^4 + 1092\eta^3 - 2010\eta^2 + 1092\eta - 3703) N^4 - 3(2461\eta^4 + 148\eta^3 \\ & - 4050\eta^2 + 148\eta + 2461) N^3 + (3839\eta^4 + 9216\eta^3 - 2190\eta^2 + 9216\eta + 3839) N^2 \\ & + (1351\eta^4 - 1032\eta^3 - 12030\eta^2 - 1032\eta + 1351) N \\ & - 6(127\eta^4 + 736\eta^3 + 930\eta^2 + 736\eta + 127) , \quad (7.203) \end{aligned}$$

$$\begin{aligned} P_{163} = & 800(\eta^4 + 1) N^8 + 8(269\eta^4 + 270\eta^3 + 270\eta + 269) N^7 - 4(589\eta^4 - 1185\eta^3 \\ & + 60\eta^2 - 1185\eta + 589) N^6 - 6(1409\eta^4 + 1438\eta^3 - 110\eta^2 + 1438\eta + 1409) N^5 \\ & + (3703\eta^4 - 1092\eta^3 + 2010\eta^2 - 1092\eta + 3703) N^4 + 3(2461\eta^4 + 148\eta^3 \\ & - 4050\eta^2 + 148\eta + 2461) N^3 - (3839\eta^4 + 9216\eta^3 - 2190\eta^2 + 9216\eta + 3839) N^2 \\ & + (-1351\eta^4 + 1032\eta^3 + 12030\eta^2 + 1032\eta - 1351) N \\ & + 6(127\eta^4 + 736\eta^3 + 930\eta^2 + 736\eta + 127) , \quad (7.204) \end{aligned}$$

$$\begin{aligned} P_{164} = & 9N^9 + 84N^8 + 723N^7 + 2137N^6 + 1907N^5 - 716N^4 - 2167N^3 - 1229N^2 \\ & - 400N - 132 , \quad (7.205) \end{aligned}$$

$$\begin{aligned} P_{165} = & 9(71\eta^2 + 134\eta + 71) N^9 + 3(1353\eta^2 + 5642\eta + 1353) N^8 \\ & + 2(3153\eta^2 + 74122\eta + 3153) N^7 - 6(767\eta^2 - 70930\eta + 767) N^6 \\ & - 3(4811\eta^2 - 119250\eta + 4811) N^5 + 3(833\eta^2 - 59782\eta + 833) N^4 \\ & + 768(19\eta^2 - 563\eta + 19) N^3 - 12(211\eta^2 + 16410\eta + 211) N^2 \\ & - 64(111\eta^2 + 899\eta + 111) N + 576(\eta^2 - 55\eta + 1) , \quad (7.206) \end{aligned}$$

$$\begin{aligned} P_{166} = & 92\eta N^{10} + (135\eta^2 + 274\eta + 135) N^9 + 4(135\eta^2 - 491\eta + 135) N^8 \\ & + (2646\eta^2 - 3740\eta + 2646) N^7 + 12(423\eta^2 - 356\eta + 423) N^6 \\ & + (4563\eta^2 - 302\eta + 4563) N^5 + 32(81\eta^2 + 112\eta + 81) N^4 \\ & + 16(54\eta^2 + 533\eta + 54) N^3 + 8328\eta N^2 + 4032\eta N + 864\eta , \quad (7.207) \end{aligned}$$

$$\begin{aligned} P_{167} = & -3(45\eta^2 + 784\eta - 45) N^{10} - 15(45\eta^2 + 784\eta - 45) N^9 \\ & - 8(135\eta^2 + 1696\eta - 135) N^8 + (-270\eta^2 + 10528\eta + 270) N^7 \\ & + 5(189\eta^2 + 2480\eta - 189) N^6 + (945\eta^2 - 52496\eta - 945) N^5 \\ & + (270\eta^2 - 36832\eta - 270) N^4 + 53664\eta N^3 + 71008\eta N^2 + 37632\eta N \\ & + 12672\eta , \quad (7.208) \end{aligned}$$

$$\begin{aligned} P_{168} = & 3(45\eta^2 - 784\eta - 45) N^{10} + 15(45\eta^2 - 784\eta - 45) N^9 \\ & + 8(135\eta^2 - 1696\eta - 135) N^8 + 2(135\eta^2 + 5264\eta - 135) N^7 \\ & + (-945\eta^2 + 12400\eta + 945) N^6 + (-945\eta^2 - 52496\eta + 945) N^5 \\ & + (-270\eta^2 - 36832\eta + 270) N^4 + 53664\eta N^3 + 71008\eta N^2 + 37632\eta N \end{aligned}$$

$$+12672\eta , \quad (7.209)$$

$$\begin{aligned} P_{169} = & 20 (405\eta^2 - 10412\eta + 405) N^{10} + (6561\eta^2 - 373928\eta + 6561) N^9 \\ & + (-37422\eta^2 + 662146\eta - 37422) N^8 + (-14175\eta^2 + 1155334\eta - 14175) N^7 \\ & + 2 (8505\eta^2 - 213523\eta + 8505) N^6 + 2 (8667\eta^2 - 495421\eta + 8667) N^5 \\ & + 10 (11907\eta^2 + 15026\eta + 11907) N^4 + 12 (7722\eta^2 + 19067\eta + 7722) N^3 \\ & - 18 (243\eta^2 - 1316\eta + 243) N^2 + 77760\eta N + 25920\eta , \end{aligned} \quad (7.210)$$

$$\begin{aligned} P_{170} = & 2052 (21\eta^2 + 31\eta + 21) N^{12} + 324 (449\eta^2 + 589\eta + 449) N^{11} \\ & + (-143289\eta^2 + 4324133\eta - 143289) N^{10} + (-619569\eta^2 + 7670353\eta - 619569) N^9 \\ & - 4 (45360\eta^2 + 86993\eta + 45360) N^8 + 2 (227529\eta^2 - 7933945\eta + 227529) N^7 \\ & - (18225\eta^2 + 21127667\eta + 18225) N^6 - (836973\eta^2 + 9493739\eta + 836973) N^5 \\ & - 50 (16605\eta^2 - 80419\eta + 16605) N^4 - 24 (11421\eta^2 - 125029\eta + 11421) N^3 \\ & - 1225440\eta N^2 - 518400\eta N + 181440\eta , \end{aligned} \quad (7.211)$$

$$\begin{aligned} P_{171} = & 12 (405\eta^2 - 3766\eta + 405) N^{14} + 48 (405\eta^2 - 3766\eta + 405) N^{13} \\ & + (8505\eta^2 + 20626\eta + 8505) N^{12} - 6 (7155\eta^2 - 116218\eta + 7155) N^{11} \\ & - (9315\eta^2 + 228902\eta + 9315) N^{10} + (322866\eta^2 - 3020828\eta + 322866) N^9 \\ & + (815427\eta^2 - 112666\eta + 815427) N^8 + (952074\eta^2 + 4787348\eta + 952074) N^7 \\ & + 45 (14967\eta^2 + 41806\eta + 14967) N^6 + 2 (162243\eta^2 - 504122\eta + 162243) N^5 \\ & + 32 (2592\eta^2 + 35513\eta + 2592) N^4 + 1629312\eta N^3 + 670752\eta N^2 \\ & + 86400\eta N - 72576\eta . \end{aligned} \quad (7.212)$$

The expression for  $\tilde{a}_{gg,Q}^{(3)}(N)$  exhibits potential poles at  $N = 1/2$  and  $N = 3/2$  due to rational pre-factors, which have to be investigated. An expansion around the corresponding values in  $N$  using `HarmonicSums` shows, after some calculation, that these poles vanish for general values of  $\eta$ . In the case  $\eta = 1$ , the corresponding result had been obtained in Ref. [366] before. For the proof in the case  $\eta \in ]0, 1]$ , 201 special replacement rules had to be derived and applied. A few of them are presented in Appendix H.2.

#### 7.2.4. The Momentum-space Solution

In  $z$ -space,  $\tilde{a}_{gg,Q}^{(3)}$  receives three contributions, the  $\delta$ -distribution, a  $+$ -distribution and a regular part, since it belongs to one of the diagonal OMEs. Their Mellin transform reads

$$\begin{aligned} \tilde{a}_{gg,Q}^{(3)}(N) = & \int_0^1 dz z^{N-1} \delta(1-z) \tilde{a}_{gg,Q}^{(3),\delta}(z) + \int_0^1 dz (z^{N-1} - 1) \tilde{a}_{gg,Q}^{(3),+}(z) \\ & + \int_0^1 dz z^{N-1} \tilde{a}_{gg,Q}^{(3),\text{reg}}(z) . \end{aligned} \quad (7.213)$$

In turn, the different terms can be obtained by a Mellin inversion:

$$\begin{aligned} \tilde{a}_{gg,Q}^{(3),\delta}(z) = & T_F^3 \left\{ \frac{32}{3} (L_1^3 + L_2^3) + \frac{64}{3} L_1 L_2 (L_1 + L_2) + 32\zeta_2 (L_1 + L_2) + \frac{128}{9} \zeta_3 \right\} \\ & + C_{FT_F}^2 \left\{ \frac{405 - 3766\eta + 405\eta^2}{81\eta} - \frac{784}{9} L_2 + \left[ -\frac{5 + 282\eta + 5\eta^2}{4\eta} \right. \right. \\ & \left. \left. + \frac{(1+\eta)(5-2\eta+5\eta^2)}{8\eta^{3/2}} \left( H_1(\sqrt{\eta}) + H_{-1}(\sqrt{\eta}) \right) \right] L_1 L_2 + \left[ \frac{5 - 422\eta + 5\eta^2}{8\eta} \right. \right. \end{aligned}$$

$$\begin{aligned}
 & -\frac{(1+\eta)(5-2\eta+5\eta^2)}{16\eta^{3/2}} \left( \text{H}_1(\sqrt{\eta}) + \text{H}_{-1}(\sqrt{\eta}) \right) \Big] (L_1^2 + L_2^2) \\
 & -\frac{(45-784\eta-45\eta^2)}{18\eta} \text{H}_0(\eta) + \frac{(1+\eta)(5-2\eta+5\eta^2)}{4\eta^{3/2}} \left[ \text{H}_0(\eta) \left( \text{H}_{0,1}(\sqrt{\eta}) \right. \right. \\
 & \left. \left. + \text{H}_{0,-1}(\sqrt{\eta}) \right) - 2 \left( \text{H}_{0,0,1}(\sqrt{\eta}) + \text{H}_{0,0,-1}(\sqrt{\eta}) \right) \right] - \frac{176}{3} \zeta_2 \Big\} \\
 + & \text{C}_{AT_F}^2 \left\{ \frac{38(21+31\eta+21\eta^2)}{135\eta} - \frac{4}{9} (L_1^3 - L_2^3) + \frac{4}{3} L_1 L_2 (L_1 - L_2) \right. \\
 & + \left[ -\frac{4-117\eta+4\eta^2}{3\eta} - \frac{16}{3} \text{H}_1(\eta) + \frac{(1+\eta)(4+11\eta+4\eta^2)}{6\eta^{3/2}} [\text{H}_1(\sqrt{\eta}) + \text{H}_{-1}(\sqrt{\eta})] \right] L_1 L_2 \\
 & + \left[ \frac{4+147\eta+4\eta^2}{6\eta} + \frac{8}{3} \text{H}_1(\eta) - \frac{(1+\eta)(4+11\eta+4\eta^2)}{12\eta^{3/2}} [\text{H}_1(\sqrt{\eta}) + \text{H}_{-1}(\sqrt{\eta})] \right] (L_1^2 + L_2^2) \\
 & + \left[ \frac{8(1-\eta^2)}{3\eta} + \frac{16}{3} \text{H}_{0,1}(\eta) - \frac{(1+\eta)(4+11\eta+4\eta^2)}{3\eta^{3/2}} [\text{H}_{0,1}(\sqrt{\eta}) + \text{H}_{0,-1}(\sqrt{\eta})] \right] (L_1 - L_2) \\
 & + \frac{62}{9} (L_1 + L_2) - \frac{13(1-\eta^2)}{45\eta} \text{H}_0(\eta) + \left[ \frac{71+134\eta+71\eta^2}{60\eta} \right. \\
 & \left. - \frac{(1+\eta)(71-46\eta+71\eta^2)}{120\eta^{3/2}} [\text{H}_{-1}(\sqrt{\eta}) + \text{H}_1(\sqrt{\eta})] \right] \text{H}_0^2(\eta) - \frac{4}{9} \text{H}_0^3(\eta) \\
 & - \frac{8}{3} \text{H}_0^2(\eta) \text{H}_1(\eta) + \frac{16}{3} \text{H}_0(\eta) \text{H}_{0,1}(\eta) + \frac{(1+\eta)(71-46\eta+71\eta^2)}{30\eta^{3/2}} \text{H}_0(\eta) \\
 & \times [\text{H}_{0,1}(\sqrt{\eta}) + \text{H}_{0,-1}(\sqrt{\eta})] - \frac{(1+\eta)(111+64\eta+111\eta^2)}{15\eta^{3/2}} [\text{H}_{0,0,1}(\sqrt{\eta}) + \text{H}_{0,0,-1}(\sqrt{\eta})] \\
 & \left. + \frac{88}{3} \zeta_2 \right\}, \tag{7.214}
 \end{aligned}$$

$$\tilde{a}_{gg,Q}^{(3),+}(z) =$$

$$\begin{aligned}
 & \text{C}_{AT_F}^2 \left\{ \frac{1}{1-z} \left[ \frac{80}{3} (L_1^3 + L_2^3) + \frac{1360}{27} (L_1^2 + L_2^2) + \frac{864}{27} \text{H}_0(\eta) (L_1^2 - L_2^2) \right. \right. \\
 & + \frac{32}{3} L_1 L_2 (L_1 + L_2) + \frac{640}{27} L_1 L_2 + \left. \left[ \frac{2752}{27} + \frac{64}{3} \text{H}_0^2(\eta) \right] (L_1 + L_2) \right. \\
 & + \left. \left[ \frac{368}{9} \text{H}_0(\eta) - \frac{32}{3} \text{H}_0(\eta) [\text{H}_0 - \text{H}_1] \right] (L_1 - L_2) - \frac{8(405-10412\eta+405\eta^2)}{729\eta} \right. \\
 & + \frac{40(1-\eta^2)}{9\eta} \text{H}_0(\eta) + \left[ -\frac{2(5-102\eta+5\eta^2)}{9\eta} + \frac{(1+\eta)(5+22\eta+5\eta^2)}{9\eta^{3/2}} \right. \\
 & \times [\text{H}_{-1}(\sqrt{\eta}) + \text{H}_1(\sqrt{\eta})] \Big] \text{H}_0^2(\eta) - \frac{32}{27} \text{H}_0^3(\eta) + \left[ \frac{352}{27} - \frac{64(1-\eta^2)}{15\eta} \text{H}_0(\eta) \right. \\
 & \left. - \frac{32}{3} \text{H}_0^2(\eta) \right] \text{H}_0 + \frac{32(1+\eta^2)}{15\eta} \text{H}_0^2 - \frac{64}{9} \text{H}_0^2(\eta) [\text{H}_1(\eta) - \frac{3}{2} \text{H}_1] \\
 & + \frac{128}{9} \text{H}_0(\eta) \text{H}_{0,1}(\eta) + \frac{64(1+\eta^2)}{15\eta} \text{H}_{0,1} - \frac{4(1+\eta)(5+22\eta+5\eta^2)}{9\eta^{3/2}} \text{H}_0(\eta) \\
 & \times [\text{H}_{0,1}(\sqrt{\eta}) + \text{H}_{0,-1}(\sqrt{\eta})] - \frac{128}{9} \text{H}_{0,0,1}(\eta) + \frac{8(1+\eta)(5+22\eta+5\eta^2)}{9\eta^{3/2}} [\text{H}_{0,0,1}(\sqrt{\eta}) \\
 & + \text{H}_{0,0,-1}(\sqrt{\eta})] - \frac{64}{27} \zeta_3 \Big] + \frac{5(1+\eta)(1-\eta+\eta^2)}{9\eta^{3/2}\pi(1-z)^{3/2}\sqrt{z}} \left[ -\text{H}_0^2(\eta) [\text{H}_{-1}(\sqrt{\eta}) + \text{H}_1(\sqrt{\eta})] \right.
 \end{aligned}$$



$$\begin{aligned}
 & +4H_0(\eta)[H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta})] - 8[H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta})] \\
 & + \frac{\zeta_2}{1-z} \left[ -\frac{32(18-175\eta+18\eta^2)}{135\eta} + \frac{112}{3}(L_1+L_2) \right] + F_1^{CA}(z) + F_+^{CA}(z) \Big\} , \tag{7.215}
 \end{aligned}$$

$$\tilde{a}_{gg,Q}^{(3),\text{reg}}(z) =$$

$$\begin{aligned}
 & C_{FT_F}^2 \left\{ (L_1^3 + L_2^3) \left[ \frac{8(1-z)(4+7z+4z^2)}{z} + 48(1+z)H_0 \right] \right. \\
 & + L_1 L_2 (L_1 + L_2) \left[ \frac{16(1-z)(4+7z+4z^2)}{3z} + 32(1+z)H_0 \right] \\
 & + (L_1^2 + L_2^2) \left[ -\frac{16(1-z)(37-140z-47z^2)}{9z} - \frac{8}{3}(-19-41z+8z^2)H_0 + \frac{136}{3}(1+z)H_0^2 \right. \\
 & \left. + \frac{16(1-z)(4+7z+4z^2)}{3z}H_1 + 32(1+z)H_{0,1}(z) - 32(1+z)\zeta_2 \right] \\
 & + (L_1^2 - L_2^2)H_0(\eta) \left[ \frac{16(1-z)(4+7z+4z^2)}{z} + 96(1+z)H_0 \right] \\
 & + L_1 L_2 \left[ -\frac{128(1-z)(1-11z-5z^2)}{9z} + \frac{64}{3}(3+5z)H_0 + \frac{64}{3}(1+z)H_0^2 \right] \\
 & + (L_1 + L_2) \left[ -\frac{32(1-z)(89-2089z-559z^2)}{81z} + \frac{16(1-z)(4+7z+4z^2)}{z}H_0^2(\eta) \right. \\
 & \left. + \left( \frac{64}{27}(184+175z-11z^2) + 96(1+z)H_0^2(\eta) \right)H_0 + \frac{8}{9}(35+77z-16z^2)H_0^2 \right. \\
 & \left. + \frac{176}{9}(1+z)H_0^3 + \left( -\frac{32(1-z)(32-85z-22z^2)}{27z} + \frac{64(1-z)(4+7z+4z^2)}{9z}H_0 \right)H_1 \right. \\
 & \left. + \frac{16(1-z)(4+7z+4z^2)}{9z}H_1^2 + \left( -\frac{64(4+2z-7z^2-2z^3)}{9z} + \frac{128}{3}(1+z)H_0 \right)H_{0,1} \right. \\
 & \left. - \frac{128}{3}(1+z)H_{0,0,1} + \frac{64}{3}(1+z)H_{0,1,1} + \left( \frac{8(60+37z-77z^2-44z^3)}{9z} \right. \right. \\
 & \left. \left. + \frac{112}{3}(1+z)H_0 \right)\zeta_2 + \frac{64}{3}(1+z)\zeta_3 \right] + (L_1 - L_2)H_0(\eta) \left[ -\frac{32(1-z)(32-85z-22z^2)}{9z} \right. \\
 & \left. + \frac{64}{3}(1+4z-2z^2)H_0 + 64(1+z)H_0^2 + \frac{32(1-z)(4+7z+4z^2)}{3z}H_1 + 64(1+z)H_{0,1} \right. \\
 & \left. - 64(1+z)\zeta_2 \right] + \frac{2(1+\eta)Q_9}{45\eta^{3/2}z} \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) \right. \right. \\
 & \left. \left. + H_{0,-1}(\sqrt{\eta}) \right) + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] + \frac{8Q_{14}}{4725\eta z}H_0(\eta) + \frac{4Q_{16}}{127575\eta z} \\
 & - \frac{16(1+\eta)Q_9}{45\pi\eta^{3/2}z}G_1(z) \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}) \right) \right. \\
 & \left. + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] - \frac{4(1+\eta)Q_7\sqrt{1-z}}{4725\pi\eta^{3/2}z^{3/2}} \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) \right. \\
 & \left. - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}) \right) + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] \\
 & \left. - \frac{77648(1-\eta^2)}{4725\eta z^{3/2}}H_0(\eta) + \frac{77648(1+\eta^2)}{4725\eta z^{3/2}} \left[ 2\ln(2) - H_1 - 2H_{-1}(\sqrt{z}) \right] \right\}
 \end{aligned}$$

7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

$$\begin{aligned}
& + \frac{4(1+\eta)\sqrt{1-z}\sqrt{z}Q_{10}}{4725\pi\eta^{3/2}} \left[ \text{H}_0^2(\eta) \left( \text{H}_{-1}(\sqrt{\eta}) + \text{H}_1(\sqrt{\eta}) \right) - 4\text{H}_0(\eta) \left( \text{H}_{0,1}(\sqrt{\eta}) \right. \right. \\
& \left. \left. + \text{H}_{0,-1}(\sqrt{\eta}) \right) + 8 \left( \text{H}_{0,0,1}(\sqrt{\eta}) + \text{H}_{0,0,-1}(\sqrt{\eta}) \right) \right] - \frac{32(1-z)(32-85z-22z^2)}{9z} \text{H}_0^2(\eta) \\
& - \frac{32(1-z)(4+7z+4z^2)}{27z} \text{H}_0^3(\eta) - \left[ \frac{8Q_{11}}{42525\eta} - \frac{16(40-40\eta^2+51z-51\eta^2z)}{45\eta} \right] \text{H}_0(\eta) \\
& - \frac{64(1+4z-2z^2)}{3} \text{H}_0^2(\eta) + \frac{64}{9}(1+z)\text{H}_0^3(\eta) \Big] \text{H}_0 + \left[ \frac{8Q_8}{405\eta} + 64(1+z)\text{H}_0^2(\eta) \right] \text{H}_0^2 \\
& + \frac{16}{81}(7+145z+16z^2)\text{H}_0^3 + \frac{56}{27}(1+z)\text{H}_0^4 - \left[ \frac{64(1-z)(4+7z+4z^2)}{9z} \text{H}_0^2(\eta) \right. \\
& \left. + \frac{128}{3}(1+z)\text{H}_0^2(\eta)\text{H}_0 \right] \text{H}_1(\eta) - \left[ \frac{8Q_{15}}{42525\eta z} - \frac{32(1-z)(4+7z+4z^2)}{3z} \text{H}_0^2(\eta) \right. \\
& \left. + \frac{128(1-z)(32-85z-22z^2)}{81z} \text{H}_0 + \frac{64(1-z)(4+7z+4z^2)}{27z} \text{H}_0^2 \right] \text{H}_1 \\
& - \left[ \frac{32(1-z)(32-85z-22z^2)}{81z} - \frac{64(1-z)(4+7z+4z^2)}{27z} \text{H}_0 \right] \text{H}_1^2 \\
& + \frac{32(1-z)(4+7z+4z^2)}{81z} \text{H}_1^3 + \left[ \frac{128(1-z)(4+7z+4z^2)}{9z} \text{H}_0(\eta) \right. \\
& \left. + \frac{256}{3}(1+z)\text{H}_0(\eta)\text{H}_0 \right] \text{H}_{0,1}(\eta) + \left[ \frac{16Q_{12}}{405\eta z} + 64(1+z)\text{H}_0^2(\eta) + \frac{128(4+5z+5z^2-8z^3)}{27z} \text{H}_0 \right. \\
& \left. - \frac{128}{9}(1+z)\text{H}_0^2 - \frac{128(1-z)(4+7z+4z^2)}{9z} \text{H}_1 \right] \text{H}_{0,1} - \frac{128}{3}(1+z)\text{H}_{0,1}^2 \\
& - \left[ \frac{128(1-z)(4+7z+4z^2)}{9z} + \frac{256}{3}(1+z)\text{H}_0 \right] \text{H}_{0,0,1}(\eta) - \left[ \frac{256(2+7z-2z^2-10z^3)}{27z} \right. \\
& \left. - \frac{1024}{9}(1+z)\text{H}_0 \right] \text{H}_{0,0,1} + \left[ \frac{128(20+16z-11z^2-22z^3)}{27z} + \frac{256}{9}(1+z)\text{H}_0 \right] \text{H}_{0,1,1} \\
& - \frac{2560}{9}(1+z)\text{H}_{0,0,0,1} + \frac{1280}{9}(1+z)\text{H}_{0,0,1,1} + \frac{128}{9}(1+z)\text{H}_{0,1,1,1} \\
& + \left[ -\frac{16Q_{13}}{405\eta z} - 64(1+z)\text{H}_0^2(\eta) + \frac{16}{27}(149+47z-88z^2)\text{H}_0 + \frac{464}{9}(1+z)\text{H}_0^2 \right. \\
& \left. + \frac{352(1-z)(4+7z+4z^2)}{27z} \text{H}_1 + \frac{704}{9}(1+z)\text{H}_{0,1} \right] \zeta_2 + \frac{2624}{45}(1+z)\zeta_2^2 \\
& + \left[ -\frac{32(44-7z-13z^2+12z^3)}{27z} + \frac{320}{9}(1+z)\text{H}_0 \right] \zeta_3 + \int_z^1 dy \left[ \frac{1}{z} F_1^{CF}(y) \right. \\
& \left. + \frac{1}{y} F_2^{CF}(y) + \frac{1}{y} \left( F_3^{CF}(y) + \frac{z}{y} F_4^{CF}(y) \right) \text{H}_0 \left( \frac{y}{z} \right) + \frac{z}{y^2} F_5^{CF}(y) + \frac{z^2}{y^3} F_6^{CF}(y) \right. \\
& \left. + \frac{\sqrt{y}}{2z^{3/2}} F_7^{CF}(y) + \left( \frac{3y^2-3y^3-3yz+3y^3z-4z^2+4y^3z^2}{3y^3} - 2(1+z)\text{H}_0 \right. \right. \\
& \left. \left. + \frac{2(y+z)\text{H}_0\left(\frac{z}{y}\right)}{y^2} \right) F_+^{CF}(y) \right] - \left( \frac{(1-z)(4+7z+4z^2)}{3z} + 2(1+z)\text{H}_0 \right) \int_0^z dy F_+^{CF}(y) \Big\} \\
& + C_{AT_F}^2 \left\{ \frac{16(4-9z+5z^2-5z^3)}{3z} (L_1^3 + L_2^3) + \frac{16(3-5z+2z^2-2z^3)}{3z} L_1 L_2 (L_1 + L_2) \right\}
\end{aligned}$$

$$\begin{aligned}
 & + (L_1^2 + L_2^2) \left[ \frac{8(383 - 485z + 323z^2 - 391z^3)}{27z} + \frac{272(1+z)}{9} H_0 + \frac{32(1-z)}{9z} H_1 \right] \\
 & + (L_1^2 - L_2^2) H_0(\eta) \left[ \frac{2(11 - 21z + 13z^2 - 16z^3)}{z} + 12z H_0 \right] \\
 & + L_1 L_2 \left[ \frac{64(25 - 31z + 19z^2 - 23z^3)}{27z} + \frac{128}{9} (1+z) H_0 - \frac{64(1-z)}{9z} H_1 \right] \\
 & + (L_1 + L_2) \left[ \frac{8(2266 - 2661z + 2277z^2 - 2914z^3)}{81z} + \frac{2(25 - 39z + 23z^2 - 32z^3)}{3z} H_0^2(\eta) \right. \\
 & + \left. \left( \frac{8}{27} (158 + 353z - 52z^2) + 12z H_0^2(\eta) \right) H_0 + \frac{176}{9} (1+z) H_0^2 \right. \\
 & + \left. \frac{8(52 - 33z + 87z^2 - 52z^3)}{27z} H_1 + \frac{128(1+z)}{9} H_{0,1} + \frac{16(21 - 50z + 13z^2 - 21z^3)}{9z} \zeta_2 \right] \\
 & + (L_1 - L_2) H_0(\eta) \left[ \frac{4(275 - 192z + 152z^2 - 288z^3)}{9z} - \frac{4(1 - 19z - 44z^2 - 16z^3)}{3z} H_0 \right. \\
 & + \left. \frac{4(22 - 38z + 17z^2)}{3z} H_1 - 8z H_{0,1} + 8z \zeta_2 \right] - \frac{4Q_{17}}{405\eta} H_0^3 + \frac{8Q_{25}}{135\eta z} H_{0,1,1} - \frac{8Q_{26}}{135\eta z} H_{0,0,1} \\
 & + \frac{16Q_{31}}{135\eta z} \zeta_3 + \frac{4Q_{34}}{405\eta z} H_1^2 + \frac{4Q_{37}}{25515\eta z} + \frac{16(1-z)}{15\eta z} H_0(\eta) H_0 H_1 - \frac{32(1-\eta^2)}{9\eta z} H_0(\eta) \\
 & - \frac{8(1647 + 4846\eta + 1647\eta^2)}{1215\eta z} H_1 - \frac{4(1+\eta)(1-10\eta+\eta^2)}{9\eta^{3/2} z} \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) \right. \\
 & \left. - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}) \right) + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] \\
 & - \frac{458(1-\eta^2)z^2}{105\eta} H_0(\eta) + \frac{8(4293 - 33236\eta + 4293\eta^2)z^2}{8505\eta} H_1 \\
 & - \frac{(1+\eta)(5+22\eta+5\eta^2)z^2}{9\eta^{3/2}} \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) \right. \\
 & \left. - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}) \right) + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] \\
 & + \frac{176(1-\eta^2)z}{15\eta} H_0(\eta) - \frac{4(603 - 4702\eta + 603\eta^2)z}{405\eta} H_1 \\
 & + \frac{(1+\eta)(11-86\eta+11\eta^2)z}{45\eta^{3/2}} \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) \right. \\
 & \left. - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}) \right) + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] \\
 & - \frac{5612(1+\eta^2)\ln(2)}{945\eta z^{3/2}} + \frac{2806(1-\eta^2)}{945\eta z^{3/2}} H_0(\eta) + \frac{2806(1+\eta^2)}{945\eta z^{3/2}} H_1 + \frac{5612(1+\eta^2)}{945\eta z^{3/2}} H_{-1}(\sqrt{z}) \\
 & - \frac{(1+\eta)Q_{38}}{1890\pi\eta^{3/2}z^{3/2}\sqrt{1-z}} \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}) \right) \right. \\
 & \left. + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] - \frac{1366(1-\eta^2)}{135\eta} H_0(\eta) + \frac{2Q_{35}}{135\eta z} H_0^2(\eta) \\
 & - \frac{32(1-2z+z^2-z^3)}{27z} H_0^3(\eta) + \left[ \frac{4Q_{28}}{8505\eta} - \frac{4Q_{22}}{45\eta} H_0(\eta) - \frac{4Q_{30}}{15\eta z} H_0^2(\eta) \right] H_0
 \end{aligned}$$

7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

$$\begin{aligned}
& + \left[ \frac{Q_{27}}{405\eta} - \frac{4(1-\eta^2)}{5\eta} H_0(\eta) \right] H_0^2 - \frac{64(1-2z+z^2-z^3)}{9z} H_0^2(\eta) H_1(\eta) \\
& + \left[ \frac{4(231+4058\eta+231\eta^2)}{405\eta} - \frac{8Q_{21}}{15\eta z} H_0^2 - \frac{8Q_{32}}{15\eta z} H_0(\eta) + \frac{4(58-106z+51z^2)}{9z} H_0^2(\eta) \right. \\
& - \left. \left( \frac{16Q_{20}}{15\eta z} H_0(\eta) - \frac{8Q_{33}}{405\eta z} \right) H_0 \right] H_1 + \frac{128(1-2z+z^2-z^3)}{9z} H_0(\eta) H_{0,1}(\eta) \\
& - \left[ \frac{8Q_{19}}{135\eta z} H_0 + \frac{16Q_{21}}{15\eta z} H_1 - \frac{8Q_{23}}{15\eta z} H_0(\eta) + \frac{2Q_{29}}{405\eta z} + 8z H_0^2(\eta) \right] H_{0,1} \\
& - \frac{128(1-2z+z^2-z^3)}{9z} H_{0,0,1}(\eta) \\
& - \frac{(1+\eta)(191+874\eta+191\eta^2)}{90\eta^{3/2}} \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) \right. \\
& \left. - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}) \right) + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] \\
& + \left[ \frac{8Q_{18}}{135\eta} H_0 - \frac{2Q_{36}}{405\eta z} + z \left( \frac{64(1-\eta^2)}{15\eta} H_0(\eta) + \frac{64(1+\eta^2)}{15\eta} H_1 \right) + \frac{8(1-\eta^2)}{15\eta} H_0(\eta) \right. \\
& \left. + 8z H_0^2(\eta) + \frac{16(1+\eta^2)(1-z)}{15\eta z} H_1 \right] \zeta_2 - \frac{4(1+\eta)Q_{24}}{45\pi\eta^{3/2}z} G_1(z) \left[ H_0^2(\eta) \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) \right. \\
& \left. - 4H_0(\eta) \left( H_{0,1}(\sqrt{\eta}) + H_{0,-1}(\sqrt{\eta}) \right) + 8 \left( H_{0,0,1}(\sqrt{\eta}) + H_{0,0,-1}(\sqrt{\eta}) \right) \right] \\
& + F_2^{CA}(z) + \int_z^1 dy \left[ \frac{1}{z} F_3^{CA}(y) - \frac{1}{y} H_0 \left( \frac{z}{y} \right) F_4^{CA}(y) + \frac{1}{y} F_5^{CA}(y) - \frac{z}{y^2} H_0 \left( \frac{z}{y} \right) F_6^{CA}(y) \right. \\
& \left. + \frac{z}{y^2} F_7^{CA}(y) + \frac{z^2}{y^3} F_8^{CA}(y) + \frac{\sqrt{y}}{2z^{3/2}} F_9^{CA}(y) - \frac{(1-y)(y-4z-4yz)}{4y^2} F_+^{CA}(y) \right] \\
& \left. - \frac{1-z+4z^2}{4z} \int_0^z dy F_+^{CA}(y) \right\}, \tag{7.216}
\end{aligned}$$

with the polynomials

$$Q_7 = 4853(\eta^2 - \eta + 1) + 6(3569\eta^2 + 15296\eta + 3569)z, \tag{7.217}$$

$$Q_8 = 40(9\eta^2 + 215\eta + 9) + (459\eta^2 + 4730\eta + 459)z - 880\eta z^2, \tag{7.218}$$

$$Q_9 = 95\eta^2 + 130\eta + 95 + 80(\eta^2 + 8\eta + 1)z + (68\eta^2 - 8\eta + 68)z^2, \tag{7.219}$$

$$\begin{aligned}
Q_{10} &= 3627\eta^2 - 22422\eta + 3627 + 40(209\eta^2 + 3130\eta + 209)z \\
&+ 840(17\eta^2 - 2\eta + 17)z^2, \tag{7.220}
\end{aligned}$$

$$\begin{aligned}
Q_{11} &= 1400(117\eta^2 - 1793\eta + 117) + 7(18873\eta^2 - 546250\eta + 18873)z \\
&+ 25(1755\eta^2 - 826\eta + 1755)z^2, \tag{7.221}
\end{aligned}$$

$$Q_{12} = 1280\eta + 40(9\eta^2 - 86\eta + 9)z + (459\eta^2 + 250\eta + 459)z^2 + 440\eta z^3, \tag{7.222}$$

$$Q_{13} = 1230\eta + 10(36\eta^2 - 551\eta + 36)z + (459\eta^2 + 1240\eta + 459)z^2 + 1570\eta z^3, \tag{7.223}$$

$$Q_{14} = (1-\eta^2)(19950 - 1400z - 3969z^2 - 4875z^3), \tag{7.224}$$

$$\begin{aligned}
Q_{15} &= -350(513\eta^2 + 454\eta + 513) + 12600(\eta^2 + 25\eta + 1)z + 63(567\eta^2 \\
&- 2150\eta + 567)z^2 + 25(1755\eta^2 - 826\eta + 1755)z^3, \tag{7.225}
\end{aligned}$$

$$\begin{aligned}
Q_{16} &= (z-1)[208(5319\eta^2 + 24500\eta + 5319) + (30861\eta^2 - 36940750\eta + 30861)z \\
&+ 25(5265\eta^2 - 377902\eta + 5265)z^2] \tag{7.226}
\end{aligned}$$

$$Q_{17} = -9\eta^2 - 760\eta - 9 + 8(18\eta^2 - 95\eta + 18)z, \tag{7.227}$$

$$Q_{18} = -9\eta^2 + 100\eta - 9 + 4(36\eta^2 + 25\eta + 36)z, \quad (7.228)$$

$$Q_{19} = -18(\eta^2 + 1) + (27\eta^2 - 320\eta + 27)z - 320\eta z^2, \quad (7.229)$$

$$Q_{20} = \eta^2 - \eta^2 z + 4(\eta^2 - 1)z^2, \quad (7.230)$$

$$Q_{21} = (\eta^2 + 1)(1 - z + 4z^2), \quad (7.231)$$

$$Q_{22} = (\eta^2 - 1)(-141 + 23z + 12z^2), \quad (7.232)$$

$$Q_{23} = (\eta^2 - 1)(2 - z + 16z^2), \quad (7.233)$$

$$Q_{24} = -24(3\eta^2 - 8\eta + 3) - (109\eta^2 + 446\eta + 109)z + 4(11\eta^2 - 86\eta + 11)z^2, \quad (7.234)$$

$$Q_{25} = 36(\eta^2 + 1) - 5(9\eta^2 - 32\eta + 9)z + 8(9\eta^2 + 20\eta + 9)z^2, \quad (7.235)$$

$$Q_{26} = 18(\eta^2 + 1) - 5(9\eta^2 - 64\eta + 9)z + 8(9\eta^2 + 40\eta + 9)z^2, \quad (7.236)$$

$$Q_{27} = -7(279\eta^2 - 538\eta + 279) + 4(153\eta^2 + 5296\eta + 153)z + 8(27\eta^2 - 520\eta + 27)z^2, \quad (7.237)$$

$$Q_{28} = 63(23\eta^2 + 2874\eta + 23) - 21(1035\eta^2 - 21322\eta + 1035)z + (8586\eta^2 - 66472\eta + 8586)z^2, \quad (7.238)$$

$$Q_{29} = 20(27\eta^2 + 208\eta + 27) + (117\eta^2 - 86\eta + 117)z + 4(117\eta^2 - 986\eta + 117)z^2 - 2080\eta z^3, \quad (7.239)$$

$$Q_{30} = 5\eta + (\eta^2 - 95\eta + 1)z + 4(2\eta^2 - 55\eta + 2)z^2 - 80\eta z^3, \quad (7.240)$$

$$Q_{31} = -20\eta - 3(3\eta^2 - 40\eta + 3)z + 12(3\eta^2 + 5\eta + 3)z^2 + 20\eta z^3, \quad (7.241)$$

$$Q_{32} = (\eta^2 - 1)(5 - 17z + 10z^2 + 2z^3), \quad (7.242)$$

$$Q_{33} = 5(27\eta^2 + 208\eta + 27) - 3(153\eta^2 + 220\eta + 153)z + 30(9\eta^2 + 26\eta + 9)z^2 + 2(27\eta^2 - 520\eta + 27)z^3, \quad (7.243)$$

$$Q_{34} = 5(27\eta^2 + 104\eta + 27) - 3(153\eta^2 + 110\eta + 153)z + 90(3\eta^2 - \eta + 3)z^2 + (54\eta^2 - 520\eta + 54)z^3, \quad (7.244)$$

$$Q_{35} = 42(\eta^2 + 159\eta + 1) - (183\eta^2 + 3088\eta + 183)z + 3(71\eta^2 + 1044\eta + 71)z^2 + (111\eta^2 - 6890\eta + 111)z^3, \quad (7.245)$$

$$Q_{36} = -19320\eta + (-1953\eta^2 + 21806\eta - 1953)z + (612\eta^2 - 8896\eta + 612)z^2 + 8(27\eta^2 + 2155\eta + 27)z^3, \quad (7.246)$$

$$Q_{37} = 7479\eta^2 + 1869560\eta + 7479 - (47655\eta^2 + 1947526\eta + 47655)z - (28593\eta^2 - 2351174\eta + 28593)z^2 + 2(55647\eta^2 - 1501024\eta + 55647)z^3, \quad (7.247)$$

$$Q_{38} = -1403(\eta^2 - \eta + 1) - (9445\eta^2 + 10652\eta + 9445)z + 3(4789\eta^2 - 10942\eta + 4789)z^2 + (278\eta^2 + 47476\eta + 278)z^3 - 4(3023\eta^2 - 5606\eta + 3023)z^4 + 336(11\eta^2 - 86\eta + 11)z^5. \quad (7.248)$$

In the above equations a series of functions,  $F_k$ , have been used. They further depend on the functions  $G_k(y)$  and  $K_k$ , which are given in Appendix H.2 and for which the  $\eta$  dependence is suppressed for brevity. The functions  $F_k$  are given by

$$F_1^{CF}(y) = \frac{16R_{14}}{9\eta^2} - \frac{16(19 + 82\eta + 19\eta^2)}{9\eta^2\sqrt{1-y}\sqrt{y}}G_1(y) \left\{ 2(1-\eta)^2 + (1-\eta^2)H_0(\eta) \right\} - \frac{16(1+\eta)^2(19+26\eta+19\eta^2)}{9\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} + \frac{4(1-\eta)^2(19-3\eta)(1+3\eta)}{9\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right\}$$

$$\begin{aligned}
 & +\mathrm{H}_0(\eta) \left[ G_4(y) - K_6 \right] + \frac{8}{\pi} \left[ K_{21} + K_{22} + K_{23} + K_{24} + \mathrm{H}_0(\eta)K_{15} \right] \Big\} \\
 & + \frac{4(1-\eta)^2(3+\eta)(3-19\eta)}{9\eta\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. -\mathrm{H}_0(\eta) \left[ G_5(y) - K_7 \right] + \frac{8}{\pi} \left[ K_{25} + K_{26} + K_{27} + K_{28} - \mathrm{H}_0(\eta)K_{18} \right] \right\} \\
 & - \frac{8R_{16}}{9\eta^2(1-y+\eta y)(-\eta-y+\eta y)} \mathrm{H}_0(\eta) - \frac{40(1+\eta)^2(19+26\eta+19\eta^2)}{27\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
 & + \frac{8R_{15}}{9\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [\mathrm{H}_0(y) + \mathrm{H}_1(y)] \\
 & + \frac{16(1+\eta)(1+\eta+\eta^2)(19+26\eta+19\eta^2)}{27(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} \mathrm{H}_0(\eta) \\
 & - \frac{4(1+\eta)^2(19+26\eta+19\eta^2)}{9(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} \mathrm{H}_0^2(\eta) + \frac{56(1-\eta^2)\pi}{9\eta\sqrt{1-y}\sqrt{y}} \mathrm{H}_0(\eta) \\
 & + \frac{2}{3\eta^2\pi\sqrt{1-y}\sqrt{y}} \zeta_2 \left\{ 2(1-\eta)^2(19+82\eta+19\eta^2) \right. \\
 & \left. + (1-\eta^2)(19+26\eta+19\eta^2)\mathrm{H}_0(\eta) \right\}, \tag{7.249}
 \end{aligned}$$

$$\begin{aligned}
 F_2^{CF}(y) = & -\frac{32R_{20}}{27\eta^2} + \frac{64(1-53\eta+\eta^2)}{27\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(1-\eta)^2 + (1-\eta^2)\mathrm{H}_0(\eta) \right\} \\
 & + \frac{64(1+\eta)^2(1+26\eta+\eta^2)}{27\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & - \frac{8(1-\eta)^2(2-9\eta)(1-9\eta)}{27\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. +\mathrm{H}_0(\eta) \left[ G_4(y) - K_6 \right] + \frac{8}{\pi} \left[ K_{21} + K_{22} + K_{23} + K_{24} + \mathrm{H}_0(\eta)K_{15} \right] \right\} \\
 & + \frac{8(1-\eta)^2(9-2\eta)(9-\eta)}{27\eta\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. -\mathrm{H}_0(\eta) \left[ G_5(y) - K_7 \right] + \frac{8}{\pi} \left[ K_{25} + K_{26} + K_{27} + K_{28} - \mathrm{H}_0(\eta)K_{18} \right] \right\} \\
 & + \frac{16R_{21}}{27\eta^2(1-y+\eta y)(-\eta-y+\eta y)} \mathrm{H}_0(\eta) + \frac{160(1+\eta)^2(1+26\eta+\eta^2)}{81\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
 & - \frac{16R_{22}}{27\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [\mathrm{H}_0(y) + \mathrm{H}_1(y)] \\
 & - \frac{64(1+\eta)(1+\eta+\eta^2)(1+26\eta+\eta^2)}{81(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} \mathrm{H}_0(\eta) \\
 & + \frac{16(1+\eta)^2(1+26\eta+\eta^2)}{27(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} \mathrm{H}_0^2(\eta) + \frac{316(1-\eta^2)\pi}{27\eta\sqrt{1-y}\sqrt{y}} \mathrm{H}_0(\eta) \\
 & - \frac{8\zeta_2}{9\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 2(-1+\eta)^2(1-53\eta+\eta^2) \right. \\
 & \left. + (1-\eta^2)(1+26\eta+\eta^2)\mathrm{H}_0(\eta) \right\}, \tag{7.250}
 \end{aligned}$$

$$\begin{aligned}
 F_3^{CF}(y) = & -\frac{128R_{17}}{9\eta^2} + \frac{128(1+10\eta+\eta^2)}{9\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(1-\eta)^2 + (1-\eta^2)H_0(\eta) \right\} \\
 & + \frac{128(1+\eta)^2(1+8\eta+\eta^2)}{9\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & - \frac{32(1-\eta)^2(1+9\eta)}{9\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + H_0(\eta) [G_4(y) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15}] \right\} \\
 & + \frac{32(1-\eta)^2(9+\eta)}{9\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - H_0(\eta) [G_5(y) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - H_0(\eta)K_{18}] \right\} \\
 & + \frac{64R_{18}}{9\eta^2(1-y+\eta y)(-\eta-y+\eta y)} H_0(\eta) + \frac{320(1+\eta)^2(1+8\eta+\eta^2)}{27\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
 & - \frac{64R_{19}}{9\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [H_0(y) + H_1(y)] \\
 & - \frac{128(1+\eta)(1+\eta+\eta^2)(1+8\eta+\eta^2)}{27(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{32(1+\eta)^2(1+8\eta+\eta^2)}{9(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} H_0^2(\eta) - \frac{16(1-\eta^2)\pi}{9\eta\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{16\zeta_2}{3\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ -2(-1+\eta)^2(1+10\eta+\eta^2) \right. \\
 & \left. - (1-\eta^2)(1+8\eta+\eta^2)H_0(\eta) \right\}, \tag{7.251}
 \end{aligned}$$

$$\begin{aligned}
 F_4^{CF}(y) = & -\frac{16R_{23}}{15\eta^2} + \frac{16(17+302\eta+17\eta^2)}{15\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(1-\eta)^2 + (1-\eta^2)H_0(\eta) \right\} \\
 & + \frac{16(1+\eta)^2(17-2\eta+17\eta^2)}{15\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & + \frac{4(1-\eta)^2(-17-150\eta+135\eta^2)}{15\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + H_0(\eta) [G_4(y) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15}] \right\} \\
 & + \frac{4(1-\eta)^2(-135+150\eta+17\eta^2)}{15\eta\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - H_0(\eta) [G_5(y) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - H_0(\eta)K_{18}] \right\} \\
 & + \frac{8R_{25}}{15\eta^2(1-y+\eta y)(-\eta-y+\eta y)} H_0(\eta) + \frac{8(1+\eta)^2(17-2\eta+17\eta^2)}{9\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
 & - \frac{8R_{24}}{15\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [H_0(y) + H_1(y)] \\
 & - \frac{16(1+\eta)(1+\eta+\eta^2)(17-2\eta+17\eta^2)}{45(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta)
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{4(1+\eta)^2(17-2\eta+17\eta^2)}{15(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}}\mathrm{H}_0(\eta)^2 - \frac{304(1-\eta^2)\pi}{15\eta\sqrt{1-y}\sqrt{y}}\mathrm{H}_0(\eta) \\
 & - \frac{2\zeta_2}{5\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 2(-1+\eta)^2(17+302\eta+17\eta^2) \right. \\
 & \left. + (1-\eta^2)(17-2\eta+17\eta^2)\mathrm{H}_0(\eta) \right\}, \tag{7.252}
 \end{aligned}$$

$$\begin{aligned}
 F_5^{CF}(y) = & -\frac{8R_{26}}{25\eta^2} + \frac{8(21+446\eta+21\eta^2)}{25\eta^2\sqrt{1-y}\sqrt{y}}G_1(y) \left\{ 2(1-\eta)^2 + (1-\eta^2)\mathrm{H}_0(\eta) \right\} \\
 & + \frac{8(1+\eta)^2(21-346\eta+21\eta^2)}{25\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} \left[ K_{19} + K_{20} \right] \right\} \\
 & + \frac{2(1-\eta)^2(-21-50\eta+375\eta^2)}{25\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + \mathrm{H}_0(\eta) \left[ G_4(y) - K_6 \right] + \frac{8}{\pi} \left[ K_{21} + K_{22} + K_{23} + K_{24} + \mathrm{H}_0(\eta)K_{15} \right] \right\} \\
 & + \frac{2(-1+\eta)^2(-375+50\eta+21\eta^2)}{25\eta\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - \mathrm{H}_0(\eta) \left[ G_5(y) - K_7 \right] + \frac{8}{\pi} \left[ K_{25} + K_{26} + K_{27} + K_{28} - \mathrm{H}_0(\eta)K_{18} \right] \right\} \\
 & + \frac{4R_{28}}{25\eta^2(1-y+\eta y)(-\eta-y+\eta y)}\mathrm{H}_0(\eta) + \frac{4(1+\eta)^2(21-346\eta+21\eta^2)}{15\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
 & - \frac{4R_{27}}{25\eta^2(1-y+\eta y)(-\eta-y+\eta y)} \left[ \mathrm{H}_0(y) + \mathrm{H}_1(y) \right] \\
 & - \frac{8(1+\eta)(1+\eta+\eta^2)(21-346\eta+21\eta^2)}{75(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}}\mathrm{H}_0(\eta) \\
 & + \frac{2(1+\eta)^2(21-346\eta+21\eta^2)}{25(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}}\mathrm{H}_0^2(\eta) - \frac{396(1-\eta^2)\pi}{25\eta\sqrt{1-y}\sqrt{y}}\mathrm{H}_0(\eta) \\
 & - \frac{3\zeta_2}{25\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 2(-1+\eta)^2(21+446\eta+21\eta^2) \right. \\
 & \left. + (1-\eta^2)(21-346\eta+21\eta^2)\mathrm{H}_0(\eta) \right\}, \tag{7.253}
 \end{aligned}$$

$$\begin{aligned}
 F_6^{CF}(y) = & -\frac{8R_{29}}{63\eta^2} + \frac{8(65+1262\eta+65\eta^2)}{63\eta^2\sqrt{1-y}\sqrt{y}}G_1(y) \left\{ 2(1-\eta)^2 + (1-\eta^2)\mathrm{H}_0(\eta) \right\} \\
 & + \frac{8(1+\eta)^2(65+502\eta+65\eta^2)}{63\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} \left[ K_{19} + K_{20} \right] \right\} \\
 & + \frac{2(1-\eta)^2(-65-882\eta+315\eta^2)}{63\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + \mathrm{H}_0(\eta) \left[ G_4(y) - K_6 \right] + \frac{8}{\pi} \left[ K_{21} + K_{22} + K_{23} + K_{24} + \mathrm{H}_0(\eta)K_{15} \right] \right\} \\
 & + \frac{2(1-\eta)^2(-315+882\eta+65\eta^2)}{63\eta\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - \mathrm{H}_0(\eta) \left[ G_5(y) - K_7 \right] + \frac{8}{\pi} \left[ K_{25} + K_{26} + K_{27} + K_{28} - \mathrm{H}_0(\eta)K_{18} \right] \right\}
 \end{aligned}$$



$$\begin{aligned}
 & + \frac{4R_{31}}{63\eta^2(1-y+\eta y)(-\eta-y+\eta y)} H_0(\eta) + \frac{20(1+\eta)^2(65+502\eta+65\eta^2)}{189\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
 & - \frac{4R_{30}}{63\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [H_0(y) + H_1(y)] \\
 & - \frac{8(1+\eta)(1+\eta+\eta^2)(65+502\eta+65\eta^2)}{189(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{2(1+\eta)^2(65+502\eta+65\eta^2)}{63(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} H_0^2(\eta) - \frac{380(1-\eta^2)\pi}{63\eta\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & - \frac{\zeta_2}{21\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 2(-1+\eta)^2(65+1262\eta+65\eta^2) \right. \\
 & \left. + (1-\eta^2)(65+502\eta+65\eta^2)H_0(\eta) \right\}, \tag{7.254}
 \end{aligned}$$

$$\begin{aligned}
 F_7^{CF}(y) = & -\frac{155296R_{32}}{4725\eta^2} + \frac{155296(1+\eta+\eta^2)}{4725\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(1-\eta)^2 + (1-\eta^2)H_0(\eta) \right\} \\
 & + \frac{155296(1+\eta)^2(1-\eta+\eta^2)}{4725\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & - \frac{38824(1-\eta)^2}{4725\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + H_0(\eta) [G_4(y) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15}] \right\} \\
 & + \frac{38824(-1+\eta)^2\eta}{4725\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - H_0(\eta) [G_5(y) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - H_0(\eta)K_{18}] \right\} \\
 & + \frac{77648R_{33}}{4725\eta^2(1-y+\eta y)(-\eta-y+\eta y)} H_0(\eta) + \frac{77648(1+\eta)^2(1-\eta+\eta^2)}{2835\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
 & - \frac{77648R_{34}}{4725\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [H_0(y) + H_1(y)] \\
 & - \frac{155296(1+\eta)(1-\eta+\eta^2)(1+\eta+\eta^2)}{14175(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{38824(1+\eta)^2(1-\eta+\eta^2)}{4725(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} H_0^2(\eta) + \frac{19412(-1+\eta)(1+\eta)\pi}{4725\eta\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & - \frac{19412\zeta_2}{1575\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 2(-1+\eta)^2(1+\eta+\eta^2) \right. \\
 & \left. + (1-\eta^2)(1-\eta+\eta^2)H_0(\eta) \right\}, \tag{7.255}
 \end{aligned}$$

$$\begin{aligned}
 F_+^{CF}(y) = & \frac{64}{3(1-y)} \left\{ -(1-\eta) [G_8(y) + G_9(y) - G_{10}(y) - G_{11}(y) \right. \\
 & \left. - (G_2(y) + G_3(y))H_0(\eta) \right] + H_0^2(\eta) \right\}, \tag{7.256}
 \end{aligned}$$

$$F_1^{CA}(z) = \frac{40R_{39}}{9\eta^2(-1+z)^2} - \frac{40(1+\eta+\eta^2)}{9\eta^2(1-z)^{3/2}\sqrt{z}} G_1(z) \left\{ 2(-1+\eta)^2 + (1-\eta^2)H_0(\eta) \right\}$$

$$\begin{aligned}
 & + \frac{40(1+\eta)^2(1-\eta+\eta^2)}{9\eta^2(1-z)^{3/2}\sqrt{z}} \left\{ G_6(z) + G_7(z) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & - \frac{10(-1+\eta)^2\eta}{9(1-z)^{3/2}\sqrt{z}} \left\{ G_{12}(z) + G_{13}(z) - K_{13} - K_{14} \right. \\
 & \left. + H_0(\eta) [G_4(z) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15}] \right\} \\
 & + \frac{10(-1+\eta)^2}{9\eta^2(1-z)^{3/2}\sqrt{z}} \left\{ G_{14}(z) + G_{15}(z) - K_{16} - K_{17} \right. \\
 & \left. - H_0(\eta) [G_5(z) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - H_0(\eta)K_{18}] \right\} \\
 & + \frac{100R_{35}}{27\eta^2\pi(1-z)^{3/2}z} + \frac{10R_{35}}{9(-1+\eta)^2\eta\pi(1-z)^{3/2}z} H_0^2(\eta) \\
 & - \frac{40R_{38}}{27(-1+\eta)\eta^2\pi(1-z)^{3/2}z(1-z+\eta z)(-\eta-z+\eta z)} H_0(\eta) \\
 & + \frac{20(-1+\eta)R_{40}}{9\eta^2(-1+z)^2(1-z+\eta z)(-\eta-z+\eta z)} H_0(\eta) \\
 & - \frac{5(-1+\eta)\pi R_{37}}{9\eta^2(1-z)^{3/2}z(1-z+\eta z)(-\eta-z+\eta z)} H_0(\eta) \\
 & + \frac{20R_{36}}{9\eta^2(1-z+\eta z)(-\eta-z+\eta z)} [H_0(z) + H_1(z)] \\
 & + \frac{5\zeta_2}{3\eta^2\pi(1-z)^{3/2}\sqrt{z}} \left\{ 2(-1+\eta)^2(1+\eta+\eta^2) \right. \\
 & \left. - (1-\eta^2)(1-\eta+\eta^2)H_0(\eta) \right\}, \tag{7.257}
 \end{aligned}$$

$$\begin{aligned}
 F_2^{CA}(z) = & - \frac{4R_{41}}{15\eta^2} + \frac{4(73+163\eta+73\eta^2)}{15\eta^2\sqrt{1-z}\sqrt{z}} G_1(z) \left\{ 2(-1+\eta)^2 + (1-\eta^2)H_0(\eta) \right\} \\
 & - \frac{4(1+\eta)^2(73+17\eta+73\eta^2)}{15\eta^2\sqrt{1-z}\sqrt{z}} \left\{ G_6(z) + G_7(z) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & + \frac{(-1+\eta)^2(90+73\eta)}{15\sqrt{1-z}\sqrt{z}} \left\{ G_{12}(z) + G_{13}(z) - K_{13} - K_{14} \right. \\
 & \left. + H_0(\eta) [G_4(z) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15}] \right\} \\
 & - \frac{(-1+\eta)^2(73+90\eta)}{15\eta^2\sqrt{1-z}\sqrt{z}} \left\{ G_{14}(z) + G_{15}(z) - K_{16} - K_{17} \right. \\
 & \left. - H_0(\eta) [G_5(z) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - H_0(\eta)K_{18}] \right\} \\
 & - \frac{2(1+\eta)^2(73+17\eta+73\eta^2)}{9\eta^2\pi\sqrt{1-z}\sqrt{z}} + \frac{2R_{42}}{45\eta^2(1-z+\eta z)(-\eta-z+\eta z)} H_0(\eta) \\
 & + \frac{4(1+\eta)(1+\eta+\eta^2)(73+17\eta+73\eta^2)}{45(-1+\eta)\eta^2\pi\sqrt{1-z}\sqrt{z}} H_0(\eta) \\
 & - \frac{(1+\eta)^2(73+17\eta+73\eta^2)}{15(-1+\eta)^2\eta\pi\sqrt{1-z}\sqrt{z}} H_0^2(\eta) - \frac{(1-\eta^2)(73+90\eta+73\eta^2)\pi}{30\eta^2\sqrt{1-z}\sqrt{z}} H_0(\eta) \\
 & + \frac{2R_{43}}{45\eta^2(1-z+\eta z)(-\eta-z+\eta z)} [H_0(z) + H_1(z)]
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{\zeta_2}{10\eta^2\pi\sqrt{1-z}\sqrt{z}} \left\{ 2(-1+\eta)^2(73+163\eta+73\eta^2) \right. \\
 & \left. -(1-\eta^2)(73+17\eta+73\eta^2)\text{H}_0(\eta) \right\}, \tag{7.258}
 \end{aligned}$$

$$\begin{aligned}
 F_3^{CA}(y) = & -\frac{4R_{44}}{45\eta^2} + \frac{8(61+226\eta+61\eta^2)}{45\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(-1+\eta)^2 + (1-\eta^2)\text{H}_0(\eta) \right\} \\
 & + \frac{32(1+\eta)^2(3-8\eta+3\eta^2)}{15\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & + \frac{(-1+\eta)^2(-97-105\eta+225\eta^2+25\eta^3)}{45\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + \text{H}_0(\eta) [G_4(y) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + \text{H}_0(\eta)K_{15}] \right\} \\
 & + \frac{(-1+\eta)^2(-25-225\eta+105\eta^2+97\eta^3)}{45\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - \text{H}_0(\eta) [G_5(y) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - \text{H}_0(\eta)K_{18}] \right\} \\
 & + \frac{16(1+\eta)^2(3-8\eta+3\eta^2)}{9\eta^2\pi\sqrt{1-y}\sqrt{y}} + \frac{2R_{46}}{135\eta^2(1-y+\eta y)(-\eta-y+\eta y)} \text{H}_0(\eta) \\
 & - \frac{32(1+\eta)(1+\eta+\eta^2)(3-8\eta+3\eta^2)}{45(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} \text{H}_0(\eta) \\
 & + \frac{8(1+\eta)^2(3-8\eta+3\eta^2)}{15(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} \text{H}_0^2(\eta) - \frac{(1-\eta^2)(25+322\eta+25\eta^2)\pi}{90\eta^2\sqrt{1-y}\sqrt{y}} \text{H}_0(\eta) \\
 & - \frac{2R_{45}}{135\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [\text{H}_0(y) + \text{H}_1(y)] \\
 & - \frac{2\zeta_2}{15\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ (-1+\eta)^2(61+226\eta+61\eta^2) \right. \\
 & \left. + 6(1-\eta^2)(3-8\eta+3\eta^2)\text{H}_0(\eta) \right\}, \tag{7.259}
 \end{aligned}$$

$$\begin{aligned}
 F_4^{CA}(y) = & \frac{R_{47}}{45\eta^2} + \frac{4(1+6\eta+\eta^2)}{5\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(-1+\eta)^2 + (1-\eta^2)\text{H}_0(\eta) \right\} \\
 & - \frac{2(1+\eta)^2(109+446\eta+109\eta^2)}{45\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & + \frac{(-1+\eta)^2(91+465\eta+645\eta^2+127\eta^3)}{180\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + \text{H}_0(\eta) [G_4(y) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + \text{H}_0(\eta)K_{15}] \right\} \\
 & - \frac{(-1+\eta)^2(127+645\eta+465\eta^2+91\eta^3)}{180\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - \text{H}_0(\eta) [G_5(y) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - \text{H}_0(\eta)K_{18}] \right\} \\
 & - \frac{(1+\eta)^2(109+446\eta+109\eta^2)}{27\eta^2\pi\sqrt{1-y}\sqrt{y}} + \frac{R_{48}}{90\eta^2(1-y+\eta y)(-\eta-y+\eta y)} \text{H}_0(\eta)
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{2(1+\eta)(1+\eta+\eta^2)(109+446\eta+109\eta^2)}{135(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} \mathbf{H}_0(\eta) \\
 & - \frac{(1+\eta)^2(109+446\eta+109\eta^2)}{90(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} \mathbf{H}_0^2(\eta) - \frac{(1-\eta^2)(127+554\eta+127\eta^2)\pi}{360\eta^2\sqrt{1-y}\sqrt{y}} \mathbf{H}_0(\eta) \\
 & + \frac{R_{49}}{90\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [\mathbf{H}_0(y) + \mathbf{H}_1(y)] \\
 & + \frac{\zeta_2}{60\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ -36(-1+\eta)^2(1+6\eta+\eta^2) \right. \\
 & \left. + (1-\eta^2)(109+446\eta+109\eta^2)\mathbf{H}_0(\eta) \right\}, \tag{7.260}
 \end{aligned}$$

$$\begin{aligned}
 F_5^{CA}(y) = & \frac{R_{50}}{135\eta^2} - \frac{4(581+1706\eta+581\eta^2)}{135\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(-1+\eta)^2 + (1-\eta^2)\mathbf{H}_0(\eta) \right\} \\
 & - \frac{2(1+\eta)^2(169-574\eta+169\eta^2)}{135\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & - \frac{(-1+\eta)^2(-1331-1845\eta+2655\eta^2+993\eta^3)}{540\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + \mathbf{H}_0(\eta) [G_4(y) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + \mathbf{H}_0(\eta)K_{15}] \right\} \\
 & - \frac{(-1+\eta)^2(-993-2655\eta+1845\eta^2+1331\eta^3)}{540\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - \mathbf{H}_0(\eta) [G_5(y) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - \mathbf{H}_0(\eta)K_{18}] \right\} \\
 & - \frac{(1+\eta)^2(169-574\eta+169\eta^2)}{81\eta^2\pi\sqrt{1-y}\sqrt{y}} + \frac{R_{51}}{270\eta^2(1-y+\eta y)(-\eta-y+\eta y)} \mathbf{H}_0(\eta) \\
 & + \frac{2(1+\eta)(1+\eta+\eta^2)(169-574\eta+169\eta^2)}{405(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} \mathbf{H}_0(\eta) \\
 & - \frac{(1+\eta)^2(169-574\eta+169\eta^2)}{270(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} \mathbf{H}_0^2(\eta) \\
 & + \frac{(1-\eta^2)(993+3986\eta+993\eta^2)\pi}{1080\eta^2\sqrt{1-y}\sqrt{y}} \mathbf{H}_0(\eta) \\
 & + \frac{R_{52}}{270\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [\mathbf{H}_0(y) + \mathbf{H}_1(y)] \\
 & + \frac{\zeta_2}{180\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 4(-1+\eta)^2(581+1706\eta+581\eta^2) \right. \\
 & \left. + (1-\eta^2)(169-574\eta+169\eta^2)\mathbf{H}_0(\eta) \right\}, \tag{7.261}
 \end{aligned}$$

$$\begin{aligned}
 F_6^{CA}(y) = & - \frac{2(1+\eta)^2(11-86\eta+11\eta^2)}{15\eta^2} + \frac{4(1+\eta)^2(11-86\eta+11\eta^2)}{15\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) \right. \\
 & \left. + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} - \frac{(1-\eta)^2(1+\eta)(11-86\eta+11\eta^2)}{30\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) \right. \\
 & \left. + G_{13}(y) - G_{14}(y) - G_{15}(y) - K_{13} - K_{14} + K_{16} + K_{17} \right. \\
 & \left. + \mathbf{H}_0(\eta) [G_4(y) + G_5(y) - K_6 - K_7] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} - K_{25}] \right\}
 \end{aligned}$$

$$\begin{aligned}
 & -K_{26} - K_{27} - K_{28} + H_0(\eta)[K_{15} + K_{18}]] \Big\} + \frac{2(1+\eta)^2(11-86\eta+11\eta^2)}{9\eta^2\pi\sqrt{1-y}\sqrt{y}} \\
 & - \frac{4(1+\eta)(1+\eta+\eta^2)(11-86\eta+11\eta^2)}{45(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{(1-\eta^2)(11-86\eta+11\eta^2)\pi}{60\eta^2\sqrt{1-y}\sqrt{y}} H_0(\eta) + \frac{R_{53}}{45\eta^2(1-y+\eta y)(-\eta-y+\eta y)} H_0(\eta) \\
 & + \frac{(1+\eta)^2(11-86\eta+11\eta^2)}{15(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} H_0^2(\eta) - \frac{(1-\eta^2)(11-86\eta+11\eta^2)\zeta_2}{10\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{R_{54}}{45\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [H_0(y) + H_1(y)] , \tag{7.262}
 \end{aligned}$$

$$\begin{aligned}
 F_7^{CA}(y) = & \frac{2R_{55}}{45\eta^2} - \frac{16(31+121\eta+31\eta^2)}{45\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(-1+\eta)^2 + (1-\eta^2)H_0(\eta) \right\} \\
 & + \frac{4(1+\eta)^2(229+506\eta+229\eta^2)}{45\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & - \frac{(-1+\eta)^2(105+375\eta+1095\eta^2+353\eta^3)}{90\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + H_0(\eta) [G_4(y) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15}] \right\} \\
 & + \frac{(-1+\eta)^2(353+1095\eta+375\eta^2+105\eta^3)}{90\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - H_0(\eta) [G_5(y) - K_7] + \frac{8}{\pi} [K_{25} + K_{26} + K_{27} + K_{28} - H_0(\eta)K_{18}] \right\} \\
 & + \frac{2(1+\eta)^2(229+506\eta+229\eta^2)}{27\eta^2\pi\sqrt{1-y}\sqrt{y}} + \frac{R_{57}}{45\eta^2(1-y+\eta y)(-\eta-y+\eta y)} H_0(\eta) \\
 & - \frac{4(1+\eta)(1+\eta+\eta^2)(229+506\eta+229\eta^2)}{135(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{(1+\eta)^2(229+506\eta+229\eta^2)}{45(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} H_0^2(\eta) + \frac{(1-\eta^2)(353+990\eta+353\eta^2)\pi}{180\eta^2\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{R_{56}}{45\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [H_0(y) + H_1(y)] \\
 & + \frac{\zeta_2}{30\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 8(-1+\eta)^2(31+121\eta+31\eta^2) \right. \\
 & \left. - (1-\eta^2)(229+506\eta+229\eta^2)H_0(\eta) \right\} , \tag{7.263}
 \end{aligned}$$

$$\begin{aligned}
 F_8^{CA}(y) = & \frac{R_{58}}{63\eta^2} + \frac{6(11+74\eta+11\eta^2)}{7\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(-1+\eta)^2 + (1-\eta^2)H_0(\eta) \right\} \\
 & - \frac{4(1+\eta)^2(163+1034\eta+163\eta^2)}{63\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & + \frac{(-1+\eta)^2(29+693\eta+4095\eta^2+623\eta^3)}{252\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + H_0(\eta) [G_4(y) - K_6] + \frac{8}{\pi} [K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15}] \right\}
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{(-1+\eta)^2(623+4095\eta+693\eta^2+29\eta^3)}{252\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - H_0(\eta) \left[ G_5(y) - K_7 \right] + \frac{8}{\pi} \left[ K_{25} + K_{26} + K_{27} + K_{28} - H_0(\eta)K_{18} \right] \right\} \\
 & -\frac{10(1+\eta)^2(163+1034\eta+163\eta^2)}{189\eta^2\pi\sqrt{1-y}\sqrt{y}} + \frac{R_{59}}{1890\eta^2(1-y+\eta y)(-\eta-y+\eta y)} H_0(\eta) \\
 & -\frac{(1-\eta^2)(623+4066\eta+623\eta^2)\pi}{504\eta^2\sqrt{1-y}\sqrt{y}} H_0(\eta) - \frac{(1+\eta)^2(163+1034\eta+163\eta^2)}{63(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} H_0^2(\eta) \\
 & + \frac{4(1+\eta)(1+\eta+\eta^2)(163+1034\eta+163\eta^2)}{189(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{R_{60}}{1890\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [H_0(y) + H_1(y)] \\
 & - \frac{\zeta_2}{42\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 27(-1+\eta)^2(11+74\eta+11\eta^2) \right. \\
 & \left. - (1-\eta^2)(163+1034\eta+163\eta^2)H_0(\eta) \right\}, \tag{7.264}
 \end{aligned}$$

$$\begin{aligned}
 F_9^{CA}(y) &= \frac{5612R_{61}}{945\eta^2} - \frac{5612(1+\eta+\eta^2)}{945\eta^2\sqrt{1-y}\sqrt{y}} G_1(y) \left\{ 2(-1+\eta)^2 + (1-\eta^2)H_0(\eta) \right\} \\
 & - \frac{5612(1+\eta)^2(1-\eta+\eta^2)}{945\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_6(y) + G_7(y) - \frac{8}{\pi} [K_{19} + K_{20}] \right\} \\
 & + \frac{1403(-1+\eta)^2}{945\eta^2\sqrt{1-y}\sqrt{y}} \left\{ G_{12}(y) + G_{13}(y) - K_{13} - K_{14} \right. \\
 & \left. + H_0(\eta) \left[ G_4(y) - K_6 \right] + \frac{8}{\pi} \left[ K_{21} + K_{22} + K_{23} + K_{24} + H_0(\eta)K_{15} \right] \right\} \\
 & - \frac{1403(-1+\eta)^2\eta}{945\sqrt{1-y}\sqrt{y}} \left\{ G_{14}(y) + G_{15}(y) - K_{16} - K_{17} \right. \\
 & \left. - H_0(\eta) \left[ G_5(y) - K_7 \right] + \frac{8}{\pi} \left[ K_{25} + K_{26} + K_{27} + K_{28} - H_0(\eta)K_{18} \right] \right\} \\
 & - \frac{2806(1+\eta)^2(1-\eta+\eta^2)}{567\eta^2\pi\sqrt{1-y}\sqrt{y}} + \frac{1403(1-\eta^2)\pi}{1890\eta\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & - \frac{1403(1+\eta)^2(1-\eta+\eta^2)}{945(-1+\eta)^2\eta\pi\sqrt{1-y}\sqrt{y}} H_0^2(\eta) - \frac{2806R_{62}}{945\eta^2(1-y+\eta y)(-\eta-y+\eta y)} H_0(\eta) \\
 & + \frac{5612(1+\eta)(1-\eta+\eta^2)(1+\eta+\eta^2)}{2835(-1+\eta)\eta^2\pi\sqrt{1-y}\sqrt{y}} H_0(\eta) \\
 & + \frac{2806R_{63}}{945\eta^2(1-y+\eta y)(-\eta-y+\eta y)} [H_0(y) + H_1(y)] \\
 & + \frac{1403\zeta_2}{630\eta^2\pi\sqrt{1-y}\sqrt{y}} \left\{ 2(-1+\eta)^2(1+\eta+\eta^2) \right. \\
 & \left. + (1-\eta^2)(1-\eta+\eta^2)H_0(\eta) \right\}, \tag{7.265}
 \end{aligned}$$

$$F_+^{CA}(y) = -\frac{64(1-\eta)}{15\eta(1-y)} \left\{ G_8(y) + G_9(y) - \eta^2 [G_{10}(y) + G_{11}(y)] \right\}$$

$$+ \frac{64(1-\eta)}{15\eta(1-y)} \left\{ G_2(y) + \eta^2 G_3(y) \right\} H_0(\eta) + \frac{32(1+\eta^2)}{15\eta(1-y)} H_0^2(\eta). \quad (7.266)$$

The additional polynomials  $R_k$  are given by

$$R_{14} = 2\eta(5\eta^2 + 54\eta + 5) + (19\eta^2 + 82\eta + 19)(\eta - 1)^2 y, \quad (7.267)$$

$$R_{15} = -2\eta^2(9\eta^2 - 82\eta + 9) - 4\eta(7\eta^4 - 20\eta^3 + 90\eta^2 - 20\eta + 7)y \\ - (\eta - 1)^2(19\eta^4 + 74\eta^3 + 198\eta^2 + 74\eta + 19)y^2 \\ + (\eta^2 - 1)^2(19\eta^2 + 26\eta + 19)y^3, \quad (7.268)$$

$$R_{16} = (\eta^2 - 1) \left[ 18\eta^2 - 10\eta(\eta^2 + 10\eta + 1)y - (\eta - 1)^2(19\eta^2 + 110\eta + 19)y^2 \right. \\ \left. + (\eta - 1)^2(19\eta^2 + 82\eta + 19)y^3 \right], \quad (7.269)$$

$$R_{17} = \eta(\eta^2 + 18\eta + 1) + (\eta^2 + 10\eta + 1)(\eta - 1)^2 y, \quad (7.270)$$

$$R_{18} = (\eta^2 - 1)y \left[ -\eta(\eta^2 + 10\eta + 1) - (\eta^2 + 11\eta + 1)(\eta - 1)^2 y \right. \\ \left. + (\eta^2 + 10\eta + 1)(\eta - 1)^2 y^2 \right], \quad (7.271)$$

$$R_{19} = 20\eta^3 - \eta(\eta^4 - 8\eta^3 + 54\eta^2 - 8\eta + 1)y \\ - (\eta - 1)^2(\eta^4 + 11\eta^3 + 36\eta^2 + 11\eta + 1)y^2 \\ + (\eta^2 - 1)^2(\eta^2 + 8\eta + 1)y^3, \quad (7.272)$$

$$R_{20} = \eta(83\eta^2 - 54\eta + 83) + 2(\eta^2 - 53\eta + 1)(\eta - 1)^2 y, \quad (7.273)$$

$$R_{21} = (\eta^2 - 1)y \left[ \eta(-83\eta^2 + 268\eta - 83) - (2\eta^2 - 185\eta + 2)(\eta - 1)^2 y \right. \\ \left. + 2(\eta^2 - 53\eta + 1)(\eta - 1)^2 y^2 \right], \quad (7.274)$$

$$R_{22} = 112\eta^3 + \eta(79\eta^4 - 110\eta^3 - 162\eta^2 - 110\eta + 79)y \\ - (\eta - 1)^2(2\eta^4 + 139\eta^3 + 54\eta^2 + 139\eta + 2)y^2 \\ + 2(\eta^2 - 1)^2(\eta^2 + 26\eta + 1)y^3, \quad (7.275)$$

$$R_{23} = -2\eta(59\eta^2 - 150\eta + 59) + (\eta - 1)^2(17\eta^2 + 302\eta + 17)y, \quad (7.276)$$

$$R_{24} = -2\eta^2(45\eta^2 - 122\eta + 45) - 8\eta(19\eta^4 - 56\eta^3 + 90\eta^2 - 56\eta + 19)y \\ - (\eta - 1)^2(17\eta^4 - 86\eta^3 + 330\eta^2 - 86\eta + 17)y^2 \\ + (\eta^2 - 1)^2(17\eta^2 - 2\eta + 17)y^3, \quad (7.277)$$

$$R_{25} = (\eta^2 - 1) \left[ 90\eta^2 + 2\eta(59\eta^2 - 286\eta + 59)y - (\eta - 1)^2(17\eta^2 + 454\eta + 17)y^2 \right. \\ \left. + (\eta - 1)^2(17\eta^2 + 302\eta + 17)y^3 \right], \quad (7.278)$$

$$R_{26} = -2\eta(177\eta^2 - 50\eta + 177) + (\eta - 1)^2(21\eta^2 + 446\eta + 21)y, \quad (7.279)$$

$$R_{27} = -2\eta^2(75\eta^2 + 154\eta + 75) + 4\eta(-99\eta^4 + 176\eta^3 + 150\eta^2 + 176\eta - 99)y \\ - (\eta - 1)^2(21\eta^4 - 658\eta^3 - 550\eta^2 - 658\eta + 21)y^2 \\ + (\eta^2 - 1)^2(21\eta^2 - 346\eta + 21)y^3, \quad (7.280)$$

$$R_{28} = (\eta^2 - 1) \left[ 2\eta(177\eta^2 - 598\eta + 177)y - (\eta - 1)^2(21\eta^2 + 842\eta + 21)y^2 \right.$$

7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

$$+150\eta^2 + (\eta - 1)^2 (21\eta^2 + 446\eta + 21) y^3 \Big] , \quad (7.281)$$

$$R_{29} = -2\eta (125\eta^2 - 882\eta + 125) + (\eta - 1)^2 (65\eta^2 + 1262\eta + 65) y , \quad (7.282)$$

$$R_{30} = -4\eta^2 (63\eta^2 - 442\eta + 63) - 4\eta (95\eta^4 - 409\eta^3 + 1260\eta^2 - 409\eta + 95) y - (\eta - 1)^2 (65\eta^4 + 382\eta^3 + 2898\eta^2 + 382\eta + 65) y^2 + (\eta^2 - 1)^2 (65\eta^2 + 502\eta + 65) y^3 , \quad (7.283)$$

$$R_{31} = (\eta^2 - 1) \left[ 2\eta (125\eta^2 - 946\eta + 125) y - (\eta - 1)^2 (65\eta^2 + 1642\eta + 65) y^2 + 252\eta^2 + (\eta - 1)^2 (65\eta^2 + 1262\eta + 65) y^3 \right] , \quad (7.284)$$

$$R_{32} = \eta^3 + \eta + (\eta - 1)^2 (\eta^2 + \eta + 1) y , \quad (7.285)$$

$$R_{33} = (\eta^2 - 1) y \left[ -\eta (\eta^2 + \eta + 1) - (\eta^2 - 1)^2 y + (\eta^2 + \eta + 1) (\eta - 1)^2 y^2 \right] , \quad (7.286)$$

$$R_{34} = 2\eta^3 - (\eta^5 + \eta^4 + \eta^2 + \eta) y - (\eta - 1)^2 (\eta^4 + 2\eta^3 + 2\eta + 1) y^2 + (\eta^2 - 1)^2 (\eta^2 - \eta + 1) y^3 , \quad (7.287)$$

$$R_{35} = (\eta^4 + \eta^3 + \eta + 1) \sqrt{z} , \quad (7.288)$$

$$R_{36} = -2 (\eta^5 + \eta) - (\eta^4 + 1) (\eta - 1)^2 z + (\eta^2 - 1)^2 (\eta^2 - \eta + 1) z^2 , \quad (7.289)$$

$$R_{37} = (\eta^3 + \eta^2 + \eta + 1) \sqrt{z} [-\eta - (\eta - 1)^2 z + (\eta - 1)^2 z^2] , \quad (7.290)$$

$$R_{38} = (\eta^5 + \eta^4 + \eta^3 + \eta^2 + \eta + 1) \sqrt{z} [-\eta - (\eta - 1)^2 z + (\eta - 1)^2 z^2] , \quad (7.291)$$

$$R_{39} = (z - 1) [1 + \eta^4 - 5\eta^4 z + 5\eta^3 z - z - 4z\eta^3(1 - z) + 4z\eta^4(1 - z) + 4\eta^4 z^2 - 4\eta^3 z^2] - z\eta(1 - z) , \quad (7.292)$$

$$R_{40} = (\eta + 1)(z - 1)^2 [-2 (\eta^3 + \eta) - (\eta^2 + 1) (\eta - 1)^2 z + (\eta^2 + \eta + 1) (\eta - 1)^2 z^2] , \quad (7.293)$$

$$R_{41} = -73\eta^4 - 90\eta^3 - 90\eta - 73 + (\eta - 1)^2 (73\eta^2 + 163\eta + 73) z , \quad (7.294)$$

$$R_{42} = (\eta^2 - 1) \left[ \eta (269\eta^2 + 220\eta + 269) + (219\eta^4 - 437\eta^3 - 491\eta^2 - 437\eta + 219) z - 3(\eta - 1)^2 (146\eta^2 + 253\eta + 146) z^2 + 3(\eta - 1)^2 (73\eta^2 + 163\eta + 73) z^3 \right] , \quad (7.295)$$

$$R_{43} = \eta (269\eta^4 + 220\eta^3 + 220\eta + 269) + (219\eta^6 - 437\eta^5 - 710\eta^4 - 100\eta^3 - 710\eta^2 - 437\eta + 219) z - 3(\eta - 1)^2 (146\eta^4 + 253\eta^3 + 180\eta^2 + 253\eta + 146) z^2 + 3 (\eta^2 - 1)^2 (73\eta^2 + 17\eta + 73) z^3 , \quad (7.296)$$

$$R_{44} = -25\eta^4 - 128\eta^3 + 210\eta^2 - 128\eta - 25 + 2(\eta - 1)^2 (61\eta^2 + 226\eta + 61) y , \quad (7.297)$$

$$R_{45} = -2\eta (75\eta^4 + 524\eta^3 - 1054\eta^2 + 524\eta + 75) - (75\eta^6 + 486\eta^5 - 2795\eta^4 + 3892\eta^3 - 2795\eta^2 + 486\eta + 75) y - 3(\eta - 1)^2 (47\eta^4 - 176\eta^3 - 30\eta^2 - 176\eta + 47) y^2 + 72 (\eta^2 - 1)^2 (3\eta^2 - 8\eta + 3) y^3 , \quad (7.298)$$

$$R_{46} = (\eta^2 - 1) \left[ 2\eta (75\eta^2 + 704\eta + 75) + 3 (25\eta^4 + 88\eta^3 - 922\eta^2 + 88\eta + 25) y - 9(\eta - 1)^2 (49\eta^2 + 258\eta + 49) y^2 + 6(\eta - 1)^2 (61\eta^2 + 226\eta + 61) y^3 \right] , \quad (7.299)$$

$$R_{47} = 127\eta^4 + 736\eta^3 + 930\eta^2 + 736\eta + 127 - 36(\eta - 1)^2 (\eta^2 + 6\eta + 1) y , \quad (7.300)$$



$$R_{48} = (\eta^2 - 1) \left[ 144\eta^2 + (127\eta^4 + 530\eta^3 - 1602\eta^2 + 530\eta + 127) y - (\eta - 1)^2 (163\eta^2 + 770\eta + 163) y^2 + 36(\eta - 1)^2 (\eta^2 + 6\eta + 1) y^3 \right], \quad (7.301)$$

$$R_{49} = 16\eta^2 (3\eta^2 + 160\eta + 3) + (127\eta^6 + 252\eta^5 - 367\eta^4 - 5336\eta^3 - 367\eta^2 + 252\eta + 127) y - 3(\eta - 1)^2 (115\eta^4 + 688\eta^3 + 1050\eta^2 + 688\eta + 115) y^2 + 2(\eta^2 - 1)^2 (109\eta^2 + 446\eta + 109) y^3, \quad (7.302)$$

$$R_{50} = -993\eta^4 - 1324\eta^3 + 3690\eta^2 - 1324\eta - 993 + 4(\eta - 1)^2 (581\eta^2 + 1706\eta + 581) y, \quad (7.303)$$

$$R_{51} = -(\eta^2 - 1) \left[ 6\eta (127\eta^2 + 1262\eta + 127) + (993\eta^4 + 1024\eta^3 - 15506\eta^2 + 1024\eta + 993) y - (\eta - 1)^2 (3317\eta^2 + 10810\eta + 3317) y^2 + 4(\eta - 1)^2 (581\eta^2 + 1706\eta + 581) y^3 \right], \quad (7.304)$$

$$R_{52} = -2\eta (381\eta^4 + 1338\eta^3 - 2966\eta^2 + 1338\eta + 381) + (-993\eta^6 + 1210\eta^5 + 8521\eta^4 - 15588\eta^3 + 8521\eta^2 + 1210\eta - 993) y + (\eta - 1)^2 (655\eta^4 + 1796\eta^3 - 2070\eta^2 + 1796\eta + 655) y^2 + 2(\eta^2 - 1)^2 (169\eta^2 - 574\eta + 169) y^3, \quad (7.305)$$

$$R_{53} = (\eta^2 - 1) \left[ -2\eta (11\eta^2 - 160\eta + 11) - (33\eta^2 - 406\eta + 33) (\eta - 1)^2 y + 3(11\eta^2 - 86\eta + 11) (\eta - 1)^2 y^2 \right], \quad (7.306)$$

$$R_{54} = -2\eta (11\eta^4 + 32\eta^3 - 470\eta^2 + 32\eta + 11) + (-33\eta^6 + 154\eta^5 + 161\eta^4 - 2100\eta^3 + 161\eta^2 + 154\eta - 33) y + 9(\eta^2 - 1)^2 (11\eta^2 - 86\eta + 11) y^2 - 6(\eta^2 - 1)^2 (11\eta^2 - 86\eta + 11) y^3, \quad (7.307)$$

$$R_{55} = -353\eta^4 - 1200\eta^3 - 750\eta^2 - 1200\eta - 353 + 8(\eta - 1)^2 (31\eta^2 + 121\eta + 31) y, \quad (7.308)$$

$$R_{56} = -4\eta (57\eta^4 + 275\eta^3 + 300\eta^2 + 275\eta + 57) + (-353\eta^6 - 296\eta^5 + 3025\eta^4 + 2960\eta^3 + 3025\eta^2 - 296\eta - 353) y + (\eta - 1)^2 (811\eta^4 + 3128\eta^3 + 3690\eta^2 + 3128\eta + 811) y^2 - 2(\eta^2 - 1)^2 (229\eta^2 + 506\eta + 229) y^3, \quad (7.309)$$

$$R_{57} = -(\eta^2 - 1) \left[ 4\eta (57\eta^2 + 155\eta + 57) + (353\eta^4 + 26\eta^3 - 2222\eta^2 + 26\eta + 353) y - (\eta - 1)^2 (601\eta^2 + 1958\eta + 601) y^2 + 8(\eta - 1)^2 (31\eta^2 + 121\eta + 31) y^3 \right], \quad (7.310)$$

$$R_{58} = 623\eta^4 + 4124\eta^3 + 1386\eta^2 + 4124\eta + 623 - 54(\eta - 1)^2 (11\eta^2 + 74\eta + 11) y, \quad (7.311)$$

$$R_{59} = (\eta^2 - 1) \left[ 28\eta (267\eta^2 + 1916\eta + 267) + 15(623\eta^4 + 2514\eta^3 - 11458\eta^2 + 2514\eta + 623) y - 15(\eta - 1)^2 (1217\eta^2 + 8062\eta + 1217) y^2 + 810(\eta - 1)^2 (11\eta^2 + 74\eta + 11) y^3 \right], \quad (7.312)$$

$$R_{60} = 4\eta (1869\eta^4 + 12404\eta^3 + 12254\eta^2 + 12404\eta + 1869) + (9345\eta^6 + 32808\eta^5$$

$$\begin{aligned}
 & -150697\eta^4 - 109312\eta^3 - 150697\eta^2 + 32808\eta + 9345)y \\
 & -45(\eta - 1)^2 (425\eta^4 + 3188\eta^3 + 3654\eta^2 + 3188\eta + 425) y^2 \\
 & +60 (\eta^2 - 1)^2 (163\eta^2 + 1034\eta + 163) y^3 , \tag{7.313}
 \end{aligned}$$

$$R_{61} = \eta^3 + \eta + (\eta - 1)^2 (\eta^2 + \eta + 1) y , \tag{7.314}$$

$$R_{62} = (\eta^2 - 1) y \left[ -\eta (\eta^2 + \eta + 1) - (\eta^2 - 1)^2 y + (\eta^2 + \eta + 1) (\eta - 1)^2 y^2 \right] , \tag{7.315}$$

$$\begin{aligned}
 R_{63} = & 2\eta^3 - (\eta^5 + \eta^4 + \eta^2 + \eta) y - (\eta - 1)^2 (\eta^4 + 2\eta^3 + 2\eta + 1) y^2 \\
 & + (\eta^2 - 1)^2 (\eta^2 - \eta + 1) y^3 . \tag{7.316}
 \end{aligned}$$

In intermediate steps of the calculation also a lot of constants, which are no multiple zeta values, appear. Some of them can be seen in Appendix H.2. They all cancel in the final result.

### 7.2.5. Numerical Results

In Figure 7.5 we compare the 3-loop two-mass effects contributing to  $A_{gg,Q}$  to the complete effect of the term proportional to the  $T_F^2$  color factor at  $\mathcal{O}(\alpha_s^3)$  due to heavy quarks for a series of  $\mu^2$  values as a function of  $z$  in the open interval  $[0, 1[$ . The contribution of the two-mass term to the whole  $T_F^2$ -contribution is significant. At lower values of  $\mu^2$  the ratio in Figure 7.5 shows a profile varying with the momentum fraction  $z$ . It flattens at large  $\mu^2$  due to the dominating logarithms and reaches values of  $\mathcal{O}(0.4)$  at  $\mu^2 \simeq 1000 \text{ GeV}^2$ . Therefore the two-mass contributions are comparable in size to the complete  $T_F^2$  contribution to the OME and cannot be neglected.

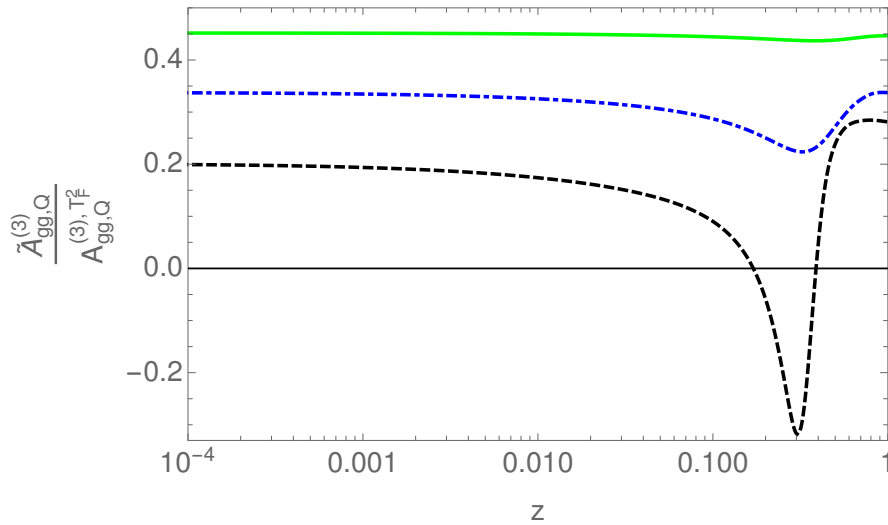


Figure 7.5.: The ratio of the two-mass (tm) contributions  $\tilde{A}_{gg,Q}^{(3)}$  to the massive OME  $A_{gg,Q}^{(3)}$  to all contributions to  $A_{gg,Q}^{(3)}$  of  $\mathcal{O}(T_F^2)$  as a function of  $z$  and  $\mu^2$ . Dashed line (black):  $\mu^2 = 50 \text{ GeV}^2$ . Dash-dotted line (blue):  $\mu^2 = 100 \text{ GeV}^2$ . Full line (green):  $\mu^2 = 1000 \text{ GeV}^2$ . Here the on-shell heavy quark masses  $m_c = 1.59 \text{ GeV}$  and  $m_b = 4.78 \text{ GeV}$  [208, 357] have been used.

### 7.3. The Operator Matrix Element $\tilde{A}_{Qg}^{(3)}$

The two mass contributions to the OME  $A_{Qg}^{(3)}$  are described by the diagrams like the ones shown in Fig. 7.6. Since the solution of the  $T_F^2$  color factor in the single mass case already includes contributions which are not first order factorizable [261] a direct calculation as for the OME  $A_{gg,Q}^{(3)}$  seems currently out of reach. Therefore we will take a different approach to the solution to this problem. Using an adapted version of the algorithm described in [367] we will calculate a large number of moments in an expansion in  $\eta$  and use guessing techniques [368, 369] to find recurrences for the different orders of the expansion.

To achieve this, the appearing loop integrals are first reduced to a small number of master integrals using Laporta's algorithm [370]. There are some publicly available programs on the market to tackle this problem [371–376]. We choose to use the package `Reduze 2`<sup>1</sup> [375]. For the set of master integrals a system of linear differential equations can be derived using the same software. Having the system of differential equations at hand the algorithm presented in [367] can be used to calculate a large number of moments, provided a sufficiently large number of initial values are known. Afterwards the guessing algorithms presented in [368, 369] can be used to find recurrences for the all  $N$  solution. If these recurrences turn out to be first-order factorizable we can find the closed form solutions with `Sigma`. From the analytic solution it is possible to transform back into momentum fraction space.

In the next section details on the steps of the calculation are given. First, the reduction to master integrals in the presence of operator insertions is discussed. Then the method to calculate arbitrary high moments in an expansion in the mass ratio  $\eta$  is addressed. Afterwards we give an algorithm based on Mellin-Barnes representations to calculate initial values directly in the  $\eta$ -expansion. With these tools at hand it is possible to calculate a large number of moments. By now 1000 moments up to  $\mathcal{O}(\eta^5)$  have been calculated, however, the last step of guessing the all  $N$  solution is still work in progress and will not be addressed in this thesis.

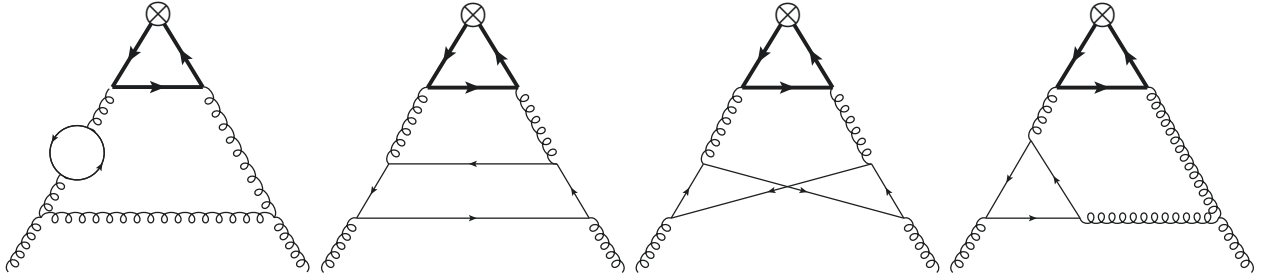


Figure 7.6.: Sample diagrams contributing to the two-mass contributions to the operator matrix element  $A_{Qg}^{(3)}$ .

#### Reduction to Master Integrals

Some sample diagrams contributing to the OME  $\tilde{A}_{Qg}^{(3)}$  can be found in Fig. 7.6. After inserting the Feynman rules, applying the appropriate projector and doing the color algebra we are left with linear combinations of integrals obeying the form

$$\int \frac{d^D k_1}{(2\pi)^D} \int \frac{d^D k_2}{(2\pi)^D} \int \frac{d^D k_3}{(2\pi)^D} \frac{\left( \prod_{i,j} (k_i \cdot k_j)^{\lambda_{i,j}} \right) \left( \prod_i (p \cdot k_i)^{\lambda_i} \right) \left( \prod_i (\Delta \cdot k_i)^{\alpha_i} \right)}{\prod_i (p_i^2 - m_i^2)} \text{OP}_\alpha^{(n)}(\tilde{p}_1, \dots, \tilde{p}_\alpha). \quad (7.317)$$

In this formula  $p$  denotes the momentum flowing through the diagram with  $p^2 = 0$ ,  $\Delta$  is an arbitrary light-like vector (i.e.  $\Delta^2 = 0$ ) and the  $\tilde{p}_i$  are linear combinations of internal and external momenta.

<sup>1</sup>`Reduze 2` uses the libraries `GiNAC` [377] and `FerMat` [378].

## 7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

Since our problem contains quarks with two different masses we have  $m_i \in (0, m_a, m_b)$ , where the massless propagators can only belong to gluons. The exponents  $\lambda_{i,j}$ ,  $\lambda_i$ ,  $\alpha_i$  and  $\nu_i$  are integers. The operator insertions can be schematically given by (cf. [379] and Appendix B)

$$\text{OP}_1^{(n)}(\tilde{p}_1) = (\Delta \cdot \tilde{p}_1)^n, \quad (7.318)$$

$$\text{OP}_2^{(n)}(\tilde{p}_1, \tilde{p}_2) = \sum_{j=0}^n (\Delta \cdot \tilde{p}_1)^j (\Delta \cdot \tilde{p}_2)^{n-j} \quad (7.319)$$

$$\text{OP}_3^{(n)}(\tilde{p}_1, \tilde{p}_2, \tilde{p}_3) = \sum_{j=0}^n \sum_{l=0}^j (\Delta \cdot \tilde{p}_1)^{n-j} (\Delta \cdot \tilde{p}_2)^{j-l} (\Delta \cdot \tilde{p}_3)^l \quad (7.320)$$

$$\text{OP}_4^{(n)}(\tilde{p}_1, \tilde{p}_2, \tilde{p}_3, \tilde{p}_4) = \sum_{j=0}^n \sum_{l=0}^j \sum_{m=0}^l (\Delta \cdot \tilde{p}_1)^{n-j} (\Delta \cdot \tilde{p}_2)^{j-l} (\Delta \cdot \tilde{p}_3)^{l-m} (\Delta \cdot \tilde{p}_4)^m \quad (7.321)$$

where  $n$  is related to the Mellin variable  $N$ . In the problem at hand the operator with four legs does not contribute. The prefactors of these integrals are polynomials of the space-time dimension  $d$ , the quark masses  $m_a$  and  $m_b$  and the scalar product of the external variables  $p \cdot \Delta$ . For the derivation of the reductions and differential equation we do not have to specify which quark is the heavier one. This, however, becomes important for the analytic solution.

Laporta's algorithm relies on Feynman integrals with propagators which have definite integer powers, the operator insertions discussed above however introduce symbolic powers in the numerator. To alleviate this problem one can formally resum the operator into a generating function. This operation transforms operator insertions into propagator-like terms by introducing a new variable  $t$ . Operator insertions involving only one momentum can for example be resummed using the geometric series

$$\sum_{N=0}^{\infty} t^N \text{OP}_1^{(N)}(\tilde{p}_1) = \sum_{N=0}^{\infty} t^N (\Delta \cdot \tilde{p}_1)^N = \frac{1}{1 - t \Delta \cdot \tilde{p}_1} \quad (7.322)$$

for propagators with more momenta the Cauchy product

$$\sum_{i=0}^{\infty} a_i \sum_{j=0}^{\infty} b_j = \sum_{i=0}^{\infty} \sum_{j=0}^i a_j b_{i-j} \quad (7.323)$$

can be used to factor the operator into two or more independent geometric series. For the operator involving two momenta we explicitly find

$$\begin{aligned} \sum_{N=0}^{\infty} t^N \text{OP}_2^{(N)}(\tilde{p}_1, \tilde{p}_2) &= \sum_{N=0}^{\infty} t^N \sum_{j=0}^N (\Delta \cdot \tilde{p}_1)^j (\Delta \cdot \tilde{p}_2)^{N-j} = \sum_{i=0}^{\infty} t^i (\Delta \cdot \tilde{p}_1)^i \sum_{i=0}^{\infty} t^j (\Delta \cdot \tilde{p}_2)^j \\ &= \frac{1}{(1 - t \Delta \cdot \tilde{p}_1)(1 - \Delta \cdot \tilde{p}_2)}. \end{aligned} \quad (7.324)$$

This procedure can be repeated recursively to also resum the operators with more attached lines into propagator-like terms

$$\sum_{N=0}^{\infty} t^N \text{OP}_3^{(N)}(\tilde{p}_1, \tilde{p}_2, \tilde{p}_3) = \frac{1}{(1 - t \Delta \cdot \tilde{p}_1)(1 - t \Delta \cdot \tilde{p}_2)(1 - \Delta \cdot \tilde{p}_3)}, \quad (7.325)$$

$$\sum_{N=0}^{\infty} t^N \text{OP}_4^{(N)}(\tilde{p}_1, \tilde{p}_2, \tilde{p}_3, \tilde{p}_4) = \frac{1}{(1 - t \Delta \cdot \tilde{p}_1)(1 - t \Delta \cdot \tilde{p}_2)(1 - t \Delta \cdot \tilde{p}_3)(1 - t \Delta \cdot \tilde{p}_4)}. \quad (7.326)$$

To find the Mellin space result, one has to expand the generating functions around  $t = 0$  and extract the  $N$ th coefficient of the series.

We need three integral families,  $B_1$ ,  $B_2$  and  $B_3$ , to cover all diagrams contributing to  $\tilde{A}_{Qg}^{(3)}$ . After resummation their respective inverse propagators are given by

$$\begin{aligned}
 P_{B_1,1} &= k_1^2 - m_a^2, & P_{B_2,1} &= k_1^2 - m_a^2, & P_{B_3,1} &= k_1^2 - m_a^2, \\
 P_{B_1,2} &= (k_1 - p)^2 - m_a^2, & P_{B_2,2} &= (k_1 - p)^2 - m_a^2, & P_{B_3,2} &= (k_1 - p)^2 - m_a^2, \\
 P_{B_1,3} &= k_2^2 - m_b^2, & P_{B_2,3} &= k_2^2 - m_b^2, & P_{B_3,3} &= k_2^2 - m_a^2, \\
 P_{B_1,4} &= (k_2 - p)^2 - m_b^2, & P_{B_2,4} &= (k_2 - p)^2 - m_b^2, & P_{B_3,4} &= (k_2 - p)^2 - m_a^2, \\
 P_{B_1,5} &= k_3^2, & P_{B_2,5} &= k_3^2, & P_{B_3,5} &= k_3^2, \\
 P_{B_1,6} &= (k_1 - k_3)^2 - m_a^2, & P_{B_2,6} &= (k_1 - k_3)^2 - m_a^2, & P_{B_3,6} &= (k_1 - k_3)^2 - m_b^2, \\
 P_{B_1,7} &= (k_2 - k_3)^2 - m_b^2, & P_{B_2,7} &= (k_2 - k_3)^2 - m_b^2, & P_{B_3,7} &= (k_2 - k_3)^2 - m_b^2, \\
 P_{B_1,8} &= (k_1 - k_2)^2, & P_{B_2,8} &= (k_1 - k_2)^2, & P_{B_3,8} &= (k_1 - k_2)^2, \\
 P_{B_1,9} &= (k_3 - p)^2, & P_{B_2,9} &= (k_3 - p)^2, & P_{B_3,9} &= (k_3 - p)^2, \\
 P_{B_1,10} &= 1 - t \Delta.k_1, & P_{B_2,10} &= 1 - t \Delta.k_1, & P_{B_3,10} &= 1 - t \Delta.k_1, \\
 P_{B_1,11} &= 1 - t \Delta.k_3, & P_{B_2,11} &= 1 - t \Delta.(k_1 - k_3), & P_{B_3,11} &= 1 - t \Delta.k_3, \\
 P_{B_1,12} &= 1 - t \Delta.k_2, & P_{B_2,12} &= 1 - t \Delta.k_2, & P_{B_3,12} &= 1 - t \Delta.k_2.
 \end{aligned} \tag{7.327}$$

Furthermore the crossed families where  $p$  goes to  $-p$  are needed for the reduction. On the moment level these integrals generally have an additional factor of  $(-1)^N$  compared to the non-crossed ones. On the level of generating functions one has to make the replacement  $t \rightarrow -t$ . The diagrams with operator insertion on an external gluon need further considerations. Here terms like

$$\frac{1}{(1 - t \Delta.k_1)(1 - t(\Delta.k_1 - \Delta.p))} \tag{7.328}$$

contribute. Since the propagators  $P_{i,10}$  to  $P_{i,12}$  do not involve the external momentum  $p$  these terms cannot be attributed to any of the integral families. However, we can use partial fractioning to obtain relations like

$$\frac{1}{(1 - t \Delta.k_1)(1 - t(\Delta.k_1 - \Delta.p))} = \frac{1}{t \Delta.p} \left( \frac{1}{1 - t \Delta.k_1} - \frac{1}{1 - t(k_1 - p)} \right). \tag{7.329}$$

The two terms can now be handled separately and mapped to one or even different integral families. Operator insertions on three and four gluons can be treated similarly and lead to three and four different terms respectively. All in all, we end up with 5168 scalar integrals which reduce to 132 master integrals using `Reduze 2` [375]. This tool also allows to derive a system of coupled differential equations for the master integrals.

### The Method of Arbitrary High Moments

This algorithm has been developed in Ref. [367]. One considers the system of coupled differential equations which can be written as

$$D_t \begin{pmatrix} I_1(t, \eta) \\ I_2(t, \eta) \\ \vdots \\ I_m(t, \eta) \end{pmatrix} = A \begin{pmatrix} I_1(t, \eta) \\ I_2(t, \eta) \\ \vdots \\ I_m(t, \eta) \end{pmatrix} + \begin{pmatrix} r_1(t, \eta) \\ r_2(t, \eta) \\ \vdots \\ r_m(t, \eta) \end{pmatrix}, \tag{7.330}$$

with  $D_t = d/dt$  and  $A$  an  $m \times m$  matrix with entries consisting of rational functions in  $\varepsilon$ ,  $\eta$  and  $t$ . This system of differential equations can be decoupled to a single higher order differential equation

## 7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

using e.g. Zürchers's algorithm [380] implemented in the package `Oresys` [381]. The master integrals  $I_j(t, \eta)$  and  $r_j(t, \eta)$  can be expanded in a Laurent expansion in  $\varepsilon$ , a Taylor series in the resummation parameter  $t$  and a logarithmically generalized Laurent series in  $\eta$ , yielding the general expressions

$$I_j(t, \eta) = \sum_{n=0}^{\infty} \left[ \sum_{k=0}^{\infty} \left( \sum_{m=0}^3 \left\{ \sum_{l=0'}^{\infty} I_j^{(k,m,l)} \ln^m(\eta) \right\} \eta^l \right) \varepsilon^k \right] t^n, \quad (7.331)$$

$$r_j(t, \eta) = \sum_{n=0}^{\infty} \left[ \sum_{k=0}^{\infty} \left( \sum_{m=0}^3 \left\{ \sum_{l=0'}^{\infty} r_j^{(k,m,l)} \ln^m(\eta) \right\} \eta^l \right) \varepsilon^k \right] t^n. \quad (7.332)$$

Inserting this ansatz into the decoupled differential equation it is possible to find recurrences for the different expansion coefficients. Provided enough initial values are known these recurrences can be used to iteratively calculate higher and higher moments of the master integrals. Although the ansatz in Eq. (7.332) generalizes the algorithm designed for single scale quantities, the generalization is rather immediate.

### An Algorithm to Calculate Initial Values in an Expansion in $\eta$

The algorithm described above needs initial values expanded to certain orders of  $\varepsilon$  and  $\eta$ . In [382] a method to calculate initial values based on dimensional shifts was introduced. Here the master integrals for fixed values of  $N$  can be reduced to a small set of scalar integrals without operator insertion in shifted dimensions. This small set of scalar integrals can then be calculated using direct integration techniques like hypergeometric methods and Mellin-Barnes integration. The drawback of this procedure is that for every higher moment the scalar integrals need to be calculated in a higher dimension, i.e. the shift  $N \rightarrow N + 1$  leads to the dimensional shift  $d \rightarrow d + 2$ .

Another method can be established using Mellin-Barnes representations of the master integrals. In the current case it was possible to find a one-dimensional Mellin-Barnes representation for all master integrals. Closing the integration contour of the Mellin-Barnes integral we end up with a linear combination of single infinite sums, which can be represented by

$$\sum_{k=0}^{\infty} \eta^{k+j \pm a\varepsilon} f(k, \varepsilon) \quad (7.333)$$

with  $j \in \mathbb{Z}$  and  $a \in (\frac{1}{2}, 1, \frac{3}{2})$ . In more involved topologies, when the operator polynomial has to be split up, further finite sums over Eq. (7.333) have to be applied. Then the function  $f(k, \varepsilon)$  will also depend on the new summation quantifiers. Fixing the value of  $N$  to an integer will lead to a collapse of the finite sums into many terms. Since we are only interested in the  $\eta$ -expansion of the initial values we can cut off the infinite sum in  $k$  to the desired order of  $\eta$ . Now only the expansion in  $\varepsilon$  has to be calculated in order to arrive at the initial values of the master integrals. The truncation of the infinite sums and high values of  $N$  will lead to a proliferation of terms. However, the last step is a simple  $\varepsilon$ -expansion of ratios of  $\Gamma$ -functions, which can be implemented very efficiently and massively parallelized, making this method of calculating initial values for the master integrals quite efficient.

For example we find

$$B_2^{1,1,1,0,0,1,1,0,0,1,1,0}(N) = \frac{iS_\varepsilon^3}{(4\pi)^6} e^{\frac{3(4-d)}{2}\gamma_E} \Gamma(5 - \frac{3d}{2}) \sum_{l=0}^N \sum_{i=0}^l \binom{l}{i} \int_0^1 dz_1 \int_0^1 dz_2 \int_0^1 dz_3 \int_0^1 dz_4 \left\{ \begin{aligned} & z_1^N [z_2(1-z_2)]^{\frac{d}{2}-2} z_3^{\frac{d}{2}-3+m} (1-z_3)^{N-m+\frac{d}{2}-2} \\ & z_4^{2+m-\frac{d}{2}} (1-z_4)^{N-l+1-\frac{d}{2}} \left[ \frac{z_4 m_1^2}{z_3(1-z_3)} + \frac{(1-z_4)m_2^2}{z_2(1-z_2)} \right]^{\frac{3d}{2}-5} \end{aligned} \right\}. \quad (7.334)$$

This allows to calculate the following first initial values up to  $\mathcal{O}(\eta^5)$ :

$$\begin{aligned}
 B_2^{(1,1,1,0,0,1,1,0,0,1,1,0),A}(0) &= \left(\frac{m_1^2}{\mu^2}\right)^{3\varepsilon/2} S_\varepsilon^3 \left\{ -\frac{1}{\varepsilon^3} \frac{8(2+\eta)}{3\eta} + \frac{1}{\varepsilon^2} \left[ \frac{8}{9\eta} + \frac{4(5+3\ln(\eta))}{3\eta} \right] \right. \\
 &+ \frac{1}{\varepsilon} \left[ -\frac{2}{3} - \zeta_2 - \frac{1}{\eta} \left( \frac{16}{3} + 2\zeta_2 + 4\ln(\eta) + \ln^2(\eta) \right) \right] - \frac{16}{3} + 2\ln(\eta) \\
 &- \ln^2(\eta) + \frac{1}{3} \ln^3(\eta) + \zeta_2 + \frac{7}{3} \zeta_3 + \frac{1}{\eta} \left( \frac{5}{3} - \frac{10}{3} \zeta_3 + \ln(\eta) - \frac{1}{6} \ln^3(\eta) \right. \\
 &+ \left. \frac{1}{2} \zeta_2 (5+3\ln(\eta)) \right) + \eta \left( \frac{7}{4} - \frac{3}{2} \ln(\eta) + \frac{1}{2} \ln^2(\eta) \right) + \eta^2 \left( \frac{19}{108} \right. \\
 &- \left. \frac{5}{18} \ln(\eta) + \frac{1}{6} \ln^2(\eta) \right) + \eta^3 \left( \frac{37}{864} - \frac{7}{72} \ln(\eta) + \frac{1}{12} \ln^2(\eta) \right) \\
 &+ \eta^4 \left( \frac{61}{4000} - \frac{9}{200} \ln(\eta) + \frac{1}{20} \ln^2(\eta) \right) \\
 &\left. + \eta^5 \left( \frac{91}{13500} - \frac{11}{450} \ln(\eta) + \frac{1}{30} \ln^2(\eta) \right) \right\} + \mathcal{O}(\eta^6 \ln^2(\eta)), \tag{7.335}
 \end{aligned}$$

$$\begin{aligned}
 B_2^{(1,1,1,0,0,1,1,0,0,1,1,0),B}(0) &= \left(\frac{m_2^2}{\mu^2}\right)^{3\varepsilon/2} S_\varepsilon^3 \left\{ -\frac{1}{\varepsilon^3} \frac{8(1+2\eta)}{3} + \frac{1}{\varepsilon^2} \left[ \frac{8}{3} + \frac{4}{3} \eta (5-3\ln(\eta)) \right] \right. \\
 &+ \frac{1}{\varepsilon} \left[ -\frac{2}{3} - \zeta_2 - \eta \left( \frac{16}{3} + 2\zeta_2 - 4\ln(\eta) + \ln(\eta)^2 \right) \right] - \frac{10}{3} + \zeta_2 + \frac{7}{3} \zeta_3 \\
 &+ \eta \left( \frac{11}{3} + \frac{1}{2} \zeta_2 (5-3\ln(\eta)) - \frac{10}{3} \zeta_3 - 3\ln(\eta) + \ln^2(\eta) - \frac{1}{6} \ln^3(\eta) \right) \\
 &+ \eta^2 \left( -\frac{7}{4} + \frac{3}{2} \ln(\eta) - \frac{1}{2} \ln^2(\eta) \right) + \eta^3 \left( -\frac{19}{108} + \frac{5}{18} \ln(\eta) - \frac{1}{6} \ln^2(\eta) \right) \\
 &+ \eta^4 \left( -\frac{37}{864} + \frac{7}{72} \ln(\eta) - \frac{1}{12} \ln^2(\eta) \right) + \eta^5 \left( -\frac{61}{4000} \right. \\
 &\left. + \frac{9}{200} \ln(\eta) - \frac{1}{20} \ln^2(\eta) \right) \left. \right\} + \mathcal{O}(\eta^6 \ln^2(\eta)), \tag{7.336}
 \end{aligned}$$

$$\begin{aligned}
 B_2^{(1,1,1,0,0,1,1,0,0,1,1,0),A}(1) &= \left(\frac{m_1^2}{\mu^2}\right)^{3\varepsilon/2} S_\varepsilon^3 \left\{ -\frac{1}{\varepsilon^3} \frac{4(3+\eta)}{3\eta} + \frac{1}{\varepsilon^2} \left[ 1 + \frac{13+9\ln(\eta)}{3\eta} \right] \right. \\
 &+ \frac{1}{\varepsilon} \left[ \frac{3}{4} - \frac{1}{2} \zeta_2 - \frac{1}{\eta} \left( \frac{11}{4} + \frac{9}{4} \ln(\eta) + \frac{3}{4} \ln^2(\eta) + \frac{3}{2} \zeta_2 \right) \right] - \frac{73}{48} - \frac{1}{2} \ln(\eta) \\
 &- \frac{1}{4} \ln^2(\eta) + \frac{1}{6} \ln^3(\eta) + \frac{3}{8} \zeta_2 + \frac{7}{6} \zeta_3 - \frac{1}{\eta} \left( \frac{23}{48} + \frac{5}{2} \zeta_3 + \frac{11}{16} \ln(\eta) \right. \\
 &+ \left. \frac{7}{16} \ln^2(\eta) + \frac{1}{8} \ln^3(\eta) - \frac{1}{8} \zeta_2 (13+9\ln(\eta)) \right) + \eta \left( \frac{415}{432} - \frac{61}{72} \ln(\eta) \right. \\
 &+ \left. \frac{7}{24} \ln^2(\eta) \right) + \eta^2 \left( \frac{913}{9000} - \frac{49}{300} \ln(\eta) + \frac{1}{10} \ln^2(\eta) \right) + \eta^3 \left( \frac{29945}{1185408} \right. \\
 &- \left. \frac{821}{14112} \ln(\eta) + \frac{17}{336} \ln^2(\eta) \right) + \eta^4 \left( \frac{53141}{5832000} - \frac{881}{32400} \ln(\eta) + \frac{11}{360} \ln^2(\eta) \right) \\
 &\left. + \eta^5 \left( \frac{97289}{23958000} - \frac{1079}{72600} \ln(\eta) + \frac{9}{440} \ln^2(\eta) \right) \right\} + \mathcal{O}(\eta^6 \ln^2(\eta)), \tag{7.337}
 \end{aligned}$$

7. Two-mass Contributions to the Unpolarized Operator Matrix Elements

$$\begin{aligned}
B_2^{(1,1,1,0,0,1,1,0,0,1,1,0),B}(1) &= \left(\frac{m_2^2}{\mu^2}\right)^{3\varepsilon/2} S_\varepsilon^3 \left\{ -\frac{1}{\varepsilon^3} \frac{4(1+3\eta)}{3} + \frac{1}{\varepsilon^2} \left[ 1 + \eta \left( \frac{13}{3} - 3 \ln(\eta) \right) \right] \right. \\
&+ \frac{1}{\varepsilon} \left[ \frac{3}{4} - \frac{1}{2} \zeta_2 - \eta \left( \frac{11}{4} - \frac{9}{4} \ln(\eta) + \frac{3}{4} \ln^2(\eta) + \frac{3}{2} \zeta_2 \right) \right] - \frac{193}{48} + \frac{3}{8} \zeta_2 \\
&+ \frac{7}{6} \zeta_3 + \eta \left( \frac{217}{48} - \frac{37}{16} \ln(\eta) + \frac{9}{16} \ln^2(\eta) - \frac{1}{8} \ln^3(\eta) + \frac{1}{8} \zeta_2 (13 - 9 \ln(\eta)) \right) \\
&- \frac{5}{2} \zeta_3 \left. \right\} + \eta^2 \left( -\frac{265}{216} + \frac{37}{36} \ln(\eta) - \frac{1}{3} \ln^2(\eta) \right) + \eta^3 \left( -\frac{6397}{54000} \right. \\
&+ \frac{331}{1800} \ln(\eta) - \frac{13}{120} \ln^2(\eta) \left. \right) + \eta^4 \left( -\frac{5585}{197568} + \frac{149}{2352} \ln(\eta) - \frac{3}{56} \ln^2(\eta) \right) \\
&+ \eta^5 \left( -\frac{116063}{11664000} + \frac{1883}{64800} \ln(\eta) - \frac{23}{720} \ln^2(\eta) \right) \left. \right\} + \mathcal{O}(\eta^6 \ln^2(\eta)). \quad (7.338)
\end{aligned}$$

**Fixed moments of  $\tilde{A}_{Qg}^{(3)}$**

Since in Ref. [202] only the irreducible contributions to the OME  $\tilde{A}_{Qg}^{(3)}$  were given, the full expressions for  $N = 2, 4, 6$  up to  $\mathcal{O}(\eta^3)$  are given in the following. These results have been computed using **Q2E** and **EXP** and provide a valuable cross check on the calculation described above.

$$\begin{aligned}
\tilde{a}_{Qg}^{(3)}(N=2) &= T_F^3 \left\{ -\frac{32}{3} (L_1^3 + L_2^3) - \frac{64}{3} L_1 L_2 (L_1 + L_2) - 32 \zeta_2 (L_1 + L_2) - \frac{128}{9} \zeta_3 \right\} \\
&+ C_{AT_F^2} \left\{ \frac{1276}{81} L_1^3 + \frac{1100}{81} L_2^3 + \frac{440}{27} L_1^2 L_2 + \frac{616}{27} L_1 L_2^2 - \frac{1090}{81} L_1^2 - \frac{1090}{81} L_2^2 \right. \\
&- \frac{1840}{81} L_1 L_2 + \frac{6844}{243} L_1 - 12 L_2 + \frac{308}{9} \zeta_2 (L_1 + L_2) + \frac{59314}{2187} - \frac{1340}{81} \zeta_2 - \frac{176}{81} \zeta_3 \\
&+ \eta \left[ \frac{256304}{10125} - \frac{7184}{675} L_\eta - \frac{8}{45} L_\eta^2 \right] + \eta^2 \left[ \frac{1565036}{496125} - \frac{6008}{4725} L_\eta - \frac{8}{45} L_\eta^2 \right] \\
&+ \eta^3 \left[ \frac{56086736}{843908625} + \frac{164464}{2679075} L_\eta - \frac{2552}{8505} L_\eta^2 \right] \left. \right\} + C_F T_F^2 \left\{ -\frac{992}{81} L_1^3 - \frac{736}{81} L_2^3 \right. \\
&- \frac{64}{27} L_1^2 L_2 - \frac{320}{27} L_1 L_2^2 + \frac{1336}{27} L_1^2 + \frac{1336}{27} L_2^2 + \frac{1936}{27} L_1 L_2 + \frac{3484}{81} L_1 + \frac{16820}{243} L_2 \\
&- \frac{160}{9} \zeta_2 (L_1 + L_2) + \frac{25556}{729} + \frac{416}{9} \zeta_2 + \frac{1408}{81} \zeta_3 + \eta \left[ -\frac{758944}{30375} - \frac{22976}{2025} L_\eta + \frac{448}{135} L_\eta^2 \right] \\
&+ \eta^2 \left[ \frac{169892864}{10418625} - \frac{1028192}{99225} L_\eta + \frac{4768}{945} L_\eta^2 \right] + \eta^3 \left[ \frac{826805984}{843908625} - \frac{5893184}{2679075} L_\eta \right. \\
&+ \left. \frac{23872}{8505} L_\eta^2 \right] \left. \right\} + \mathcal{O}(\eta^4 \ln^3(\eta)) \quad (7.339)
\end{aligned}$$

$$\begin{aligned}
\tilde{a}_{Qg}^{(3)}(N=4) &= T_F^3 \left\{ -\frac{88}{15} (L_1^3 + L_2^3) - \frac{176}{15} L_1 L_2 (L_1 + L_2) - \frac{88}{5} \zeta_2 (L_1 + L_2) - \frac{352}{45} \zeta_3 \right\} \\
&+ C_{AT_F^2} \left\{ \frac{37642}{2025} L_1^3 + \frac{1298}{81} L_2^3 + \frac{2596}{135} L_1^2 L_2 + \frac{18172}{675} L_1 L_2^2 + \frac{48311}{2700} L_1^2 + \frac{48311}{2700} L_2^2 \right. \\
&+ \frac{60304}{3375} L_1 L_2 + \frac{111162031}{1215000} L_1 + \frac{16979653}{405000} L_2 + \frac{4366284317}{36450000} + \frac{9086}{225} \zeta_2 (L_1 + L_2) \\
&+ \frac{120721}{6750} \zeta_2 - \frac{5192}{2025} \zeta_3 + \eta \left[ \frac{496855133}{14883750} - \frac{1877399}{141750} L_\eta + \frac{707}{2700} L_\eta^2 \right] \\
&+ \eta^2 \left[ \frac{1255194149}{468838125} - \frac{1634774}{1488375} L_\eta - \frac{142}{525} L_\eta^2 \right] + \eta^3 \left[ \frac{250077164867}{11232423798750} \right.
\end{aligned}$$



$$\begin{aligned}
 & \left. + \frac{156082853}{3241680750} L_\eta - \frac{744283}{1871100} L_\eta^2 \right\} + C_F T_F^2 \left\{ -\frac{360041}{40500} L_1^3 - \frac{285637}{40500} L_2^3 \right. \\
 & - \frac{33209}{6750} L_1^2 L_2 - \frac{70411}{6750} L_1 L_2^2 + \frac{2998861}{162000} L_1^2 + \frac{2998861}{162000} L_2^2 + \frac{2910757}{101250} L_1 L_2 \\
 & + \frac{42554063}{4860000} L_1 + \frac{209724793}{8100000} L_2 - \frac{70411}{4500} \zeta_2 (L_1 + L_2) - \frac{12930316237}{2187000000} + \frac{78397}{10125} \zeta_3 \\
 & + \frac{6503111}{405000} \zeta_2 + \eta \left[ -\frac{59657237}{4134375} - \frac{184214}{39375} L_\eta + \frac{2228}{1125} L_\eta^2 \right] + \eta^2 \left[ \frac{582667691}{75014100} \right. \\
 & \left. - \frac{2876423}{595350} L_\eta + \frac{27101}{9450} L_\eta^2 \right] + \eta^3 \left[ \frac{23024568781}{44929695195} - \frac{285046646}{324168075} L_\eta + \frac{879808}{467775} L_\eta^2 \right] \left. \right\} \\
 & + \mathcal{O}(\eta^4 \ln^3(\eta)) \tag{7.340}
 \end{aligned}$$

$$\begin{aligned}
 \tilde{a}_{Qg}^{(3)}(N=6) &= T_F^3 \left\{ -\frac{88}{21} (L_1^3 + L_2^3) - \frac{176}{21} L_1 L_2 (L_1 + L_2) - \frac{88}{7} \zeta_2 (L_1 + L_2) - \frac{352}{63} \zeta_3 \right\} \\
 & + C_A T_F^2 \left\{ \frac{128557}{7938} L_1^3 + \frac{110825}{7938} L_2^3 + \frac{22165}{1323} L_1^2 L_2 + \frac{4433}{189} L_1 L_2^2 + \frac{11852567}{555660} L_1^2 \right. \\
 & + \frac{11852567}{555660} L_2^2 + \frac{649960}{27783} L_1 L_2 + \frac{10225023539}{116688600} L_1 + \frac{119576963}{2593080} L_2 \\
 & + \frac{4433}{126} \zeta_2 (L_1 + L_2) + \frac{8699108665601}{73513818000} + \frac{6117389}{277830} \zeta_2 - \frac{8866}{3969} \zeta_3 \\
 & + \eta \left[ \frac{832369820129}{29172150000} - \frac{1406143531}{138915000} L_\eta + \frac{112669}{1323000} L_\eta^2 \right] + \eta^2 \left[ \frac{755537213056}{624023544375} \right. \\
 & \left. - \frac{105157957}{360186750} L_\eta - \frac{49373}{103950} L_\eta^2 \right] + \eta^3 \left[ -\frac{84840004938801319}{1381947564807810000} \right. \\
 & \left. + \frac{2287164970759}{15339633309000} L_\eta - \frac{31340489}{68108040} L_\eta^2 \right] \left. \right\} + C_F T_F^2 \left\{ -\frac{1106501}{138915} L_1^3 - \frac{25223}{3969} L_2^3 \right. \\
 & - \frac{43142}{9261} L_1^2 L_2 - \frac{439406}{46305} L_1 L_2^2 + \frac{8653111}{1080450} L_1^2 + \frac{8653111}{1080450} L_2^2 + \frac{23611796}{1620675} L_1 L_2 \\
 & - \frac{12389796287}{2042050500} L_1 + \frac{4267683493}{408410100} L_2 - \frac{219703}{15435} \zeta_2 (L_1 + L_2) - \frac{9883289655671}{428830605000} \\
 & + \frac{29196929}{4862025} \zeta_2 + \frac{130108}{19845} \zeta_3 + \eta \left[ -\frac{32427817736}{2552563125} - \frac{64271512}{24310125} L_\eta + \frac{376216}{231525} L_\eta^2 \right] \\
 & + \eta^2 \left[ \frac{524351089261}{97070329125} - \frac{11478584}{3361743} L_\eta + \frac{88972}{40425} L_\eta^2 \right] + \eta^3 \left[ \frac{990283034941336}{2467763508585375} \right. \\
 & \left. - \frac{1255768040}{2191376187} L_\eta + \frac{63929464}{42567525} L_\eta^2 \right] \left. \right\} + \mathcal{O}(\eta^4 \ln^3(\eta)) \tag{7.341}
 \end{aligned}$$

## Results and Outlook

With the algorithm described above we calculated the first 1000 moments of the OME  $\tilde{A}_{Qg}^{(3)}$  up to  $\mathcal{O}(\eta^5)$ . The poles of the unrenormalized OME are in full agreement with the expectation from renormalization, cf. Eq. (5.108). Furthermore, we agree with the moments  $N = 2, 4, 6$  previously obtained up to  $\mathcal{O}(\eta^3)$  using Q2E and EXP in Ref. [202]. Note that there only the irreducible contributions are given. In Figure 7.7 the ratio of two mass contributions over the full  $\mathcal{O}(T_F^2)$  contributions to the OME  $A_{Qg}^{(3)}$  are plotted for the fixed values of  $N = 2, 4, 6, 8, 10$ . We used the single mass contributions calculated in Ref. [359]. The ratio gets flatter for increasing  $Q^2$  and approaches 0.45 from above. It is evident that the two mass contributions are non-negligible over the whole energy range.

In a next step it might be possible to guess recurrences of the coefficients multiplying different analytic structures, which has been successfully been applied to single scale processes, cf. Refs. [261,

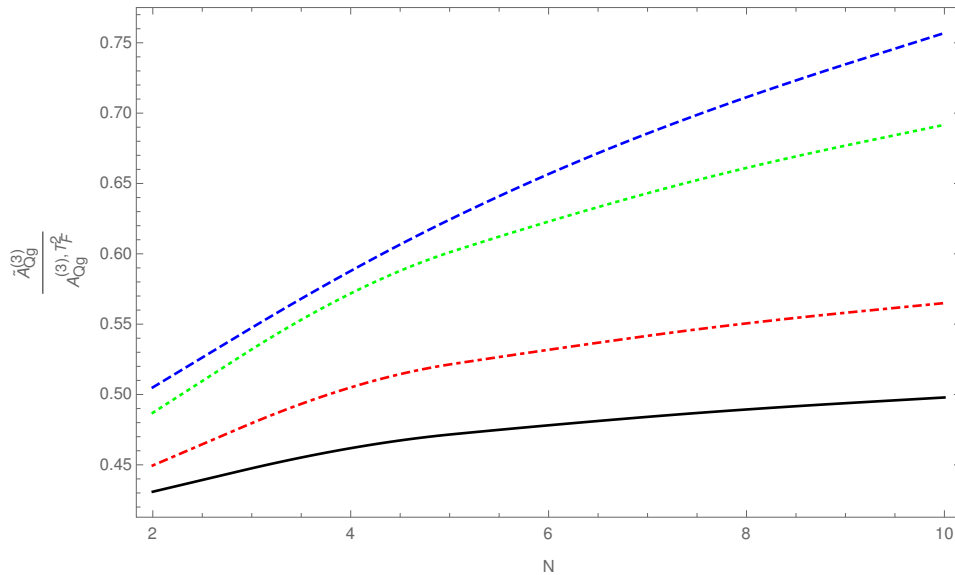


Figure 7.7.: The ratio of the two-mass contributions  $\tilde{A}_{Qg}^{(3)}$  to the full OME  $A_{Qg}^{(3)}$  of  $\mathcal{O}(T_F^2)$  for the moments  $N = 2, 4, 6, 8, 10$  as function of  $\mu^2$ . Dashed line (blue):  $\mu^2 = 50 \text{ GeV}^2$ . Dotted line (green):  $\mu^2 = 100 \text{ GeV}^2$ . Dash-dotted line (red):  $\mu^2 = 1000 \text{ GeV}^2$ . Full line (black):  $\mu^2 = 10000 \text{ GeV}^2$ . Here the on-shell heavy quark masses  $m_c = 1.59 \text{ GeV}$  and  $m_b = 4.78 \text{ GeV}$  [208, 357] have been used. The discrete points have been connected using second-order polynomials.

368], using the algorithms implemented in the publicly available software **guess** [369]. If the resulting recurrences turn out to be first order factorizable a closed form solution for general values of  $N$  will be achievable.

The procedure outlined above is well defined in Mellin space. Therefore experimental applications are presently possible in Mellin- $N$  space, requiring measured Mellin moments of the structure function  $F_2(x, Q^2)$ . Analyses of this kind, at lower order in the coupling constant, have been performed already early, e.g. in Refs. [217, 383–388]. The calculation of the all- $N$  solution and numerical studies will be left for future work.

## 8. Calculation of Polarized Massive Operator Matrix Elements

This chapter is dedicated to the calculation of massive OMEs for polarized scattering. Since the OMEs are not finite and need renormalization we have to deal with  $\gamma_5$  in  $d = 4 + \varepsilon$  dimensions. In the following this will be done in the Larin scheme. Afterwards a finite renormalization is applied to the anomalous dimensions and Wilson coefficients to arrive at the  $M$ -scheme, defined in Ref. [152]. However, there are subtleties in the calculation of the OMEs which have to be addressed first.

Like in the case of unpolarized quantities, we can extract the color, Dirac and Lorentz structure from the amputated Green's functions, cf. Eqs. (2.79-2.81). In the case of polarized scattering the identities read

$$\Delta \hat{G}_{kg,\mu\nu}^{ab} \stackrel{d=4}{=} \Delta \hat{A}_{kg} \delta^{ab} \varepsilon_{\mu\nu\alpha\beta} \Delta^\alpha p^\beta (p.\Delta)^{N-1}, \quad (8.1)$$

$$\Delta \hat{G}_{kq}^{ij} \stackrel{d=4}{=} \Delta \hat{A}_{kq} \delta^{ij} \not{\Delta} \gamma_5 (p.\Delta)^{N-1}, \quad (8.2)$$

with  $k = Q, q, g$ . As has been mentioned in Ref. [155] the tensor structures in Eqs. (8.1, 8.2) have to be understood in  $d = 4$  dimensions. Since the tensor structure in Eq. (8.1) is unique, it can be continued into  $d = 4 + \varepsilon$  dimensions unambiguously within the Larin scheme. Therefore we can use the projector

$$\Delta P_g = \frac{\delta^{ab}}{N_c^2 - 1} \frac{1}{(d-2)(d-3)} \varepsilon^{\mu\nu\rho\sigma} p_\rho \Delta_\sigma (p.\Delta)^{-N-1} \quad (8.3)$$

to extract the polarized OMEs with external gluonic legs in the Larin scheme. It has already been used in Refs. [173, 175, 176]. This is not the case for the OMEs with external quarks. In continued space time dimensions the tensor structure  $\not{\Delta} \gamma_5$  is not unique. The most general decomposition for on-shell external legs  $p^2 = 0^1$  reads

$$\Delta \hat{G}_{kq}^{ij} = \Delta \hat{A}_{iq}^{(a)} \delta^{ij} \frac{i}{6} \gamma_\mu \gamma_\nu \gamma_\rho \varepsilon^{\mu\nu\rho\Delta} (p.\Delta)^{N-1} - \Delta \hat{A}_{iq}^{(b)} \delta^{ij} \frac{i}{2} \gamma_\mu \not{\Delta} \gamma_\nu \varepsilon^{\mu\nu\rho\Delta} (p.\Delta)^{N-2}. \quad (8.4)$$

A term proportional to  $\not{p}$  does not contribute, because of the equation of motion  $\not{p}|p\rangle = 0$ . Additional terms involving  $\not{\Delta}$  do not contribute, since commuting them with the other  $\gamma$  matrices either contract the  $\varepsilon$ -tensor with an additional  $\Delta$  making it vanish because of its complete asymmetry or finally the term  $\not{\Delta} \not{\Delta} = \Delta^2 = 0$  emerges. The two tensor structures are chosen in such a way that the desired tensor structure is recovered in  $d = 4$  dimensions

$$\frac{i}{6} \gamma_\mu \gamma_\nu \gamma_\rho \varepsilon^{\mu\nu\rho\Delta} (p.\Delta)^{N-1} \stackrel{d=4}{=} \not{\Delta} \gamma_5 (p.\Delta)^{N-1}, \quad (8.5)$$

$$\frac{-i}{2} \gamma_\mu \not{\Delta} \gamma_\nu \varepsilon^{\mu\nu\rho\Delta} (p.\Delta)^{N-2} \stackrel{d=4}{=} \not{\Delta} \gamma_5 (p.\Delta)^{N-1}. \quad (8.6)$$

Since we want to treat the external tensor structures as four dimensional we are interested in

$$\Delta \hat{A}_{kq} = \Delta \hat{A}_{kq}^{(a)} + \Delta \hat{A}_{kq}^{(b)}. \quad (8.7)$$

<sup>1</sup>A third tensor structure appears for off-shell quantities.

If we now apply the projector proposed in Ref. [176]<sup>2</sup>

$$P_q^{\text{old}} \Delta \hat{G}_{kq}^{ij} = -\frac{\delta^{ij}}{N_c} \frac{3}{2(d-1)(d-2)(d-3)} \text{tr} \left[ \not{p} \gamma_5 \Delta \hat{G}_{kq}^{ij} \right] (p \cdot \Delta)^{-N} \quad (8.8)$$

we arrive at

$$\begin{aligned} P_q^{\text{old}} \Delta \hat{G}_{kq} &= -\frac{1}{N_c} \delta^{ij} \frac{3}{2(d-1)(d-2)(d-3)} \text{tr} \left[ \not{p} \gamma_5 \Delta \hat{G}_{kq}^{ij} \right] (p \cdot \Delta)^{-N} \\ &= -i \frac{\delta^{ij}}{N_c} \frac{3}{48(d-1)(d-2)(d-3)} \varepsilon_{\mu\nu\rho\sigma} \text{tr} \left[ \not{p} \gamma^\mu \gamma^\nu \gamma^\rho \gamma^\sigma \Delta \hat{G}_{kq}^{ij} \right] (p \cdot \Delta)^{-N} \\ &= \hat{A}_{kq}^{(a)} + \frac{3}{d-1} \hat{A}_{kq}^{(b)}. \end{aligned} \quad (8.9)$$

We see that both tensor structures do not enter with the same weight but mix at  $\mathcal{O}(\varepsilon)$ , the structure in Eq. (8.7) is therefore not reproduced. In Ref. [176, 302] this problem was encountered and solved by first making the structure in Eq. (8.4) manifest. This was achieved by directly computing the amputated Green's function using tensor integrals. In a last step the projector in Eq. (8.8) was applied in  $d = 4$  dimensions. This has the effect of setting  $d = 4$  in the last line of Eq. (8.9) and therefore reproduces the relation in Eq. (8.7).

However, resorting to tensorial integrals or tensorial reduction as advocated in Ref. [155] is not necessary, since using the modified projector

$$\begin{aligned} P_q \Delta \hat{G}_{kq}^{ij} &= -\frac{\delta^{ij}}{N_c} \frac{i}{4(d-2)(d-3)} \varepsilon_{\mu\nu p \Delta} \text{tr} \left[ \not{p} \gamma^\mu \gamma^\nu \Delta \hat{G}_{kq}^{ij} \right] (p \cdot \Delta)^{-N-1} \\ &= \hat{A}_{iq}^{(a)} + \hat{A}_{iq}^{(b)}, \end{aligned} \quad (8.10)$$

directly reproduces the relation given in Eq. (8.7). The projector in Eq. (8.10) is determined using the tensor structure of the amputated Green's function only and is valid for arbitrary loop orders.

The projector introduced in Eq. (8.10) now allows to compute OMEs in the polarized case in the same way as the unpolarized ones without resorting to tensor decomposition. With the projectors for gluonic and quarkonic external states at hand, the calculation of the polarized OMEs in the Larin scheme follows closely the one for unpolarized OMEs. In the following sections we will present missing pieces of the calculation of polarized OMEs at NLO and first results obtained at NNLO. Our new results at NNLO provide an independent cross check of the NLO polarized anomalous dimensions already obtained in Refs. [155–158] and the first cross check for the  $\mathcal{O}(T_F^2)$  contributions to the NNLO ones obtained in Ref. [158] in the context of a massive calculation. In the polarized case the OMEs and anomalous dimensions are only defined for odd values of the Mellin variable  $N$ . A factor  $\frac{1-(-1)^N}{2}$  is therefore always to be understood implicitly.

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<sup>2</sup>Note that in Ref. [173] no details of the calculation involving OMEs with external quarks are mentioned.

## 8.1. Finite Renormalization

The splitting functions and Wilson coefficients calculated in the Larin-scheme need a finite renormalization in order to arrive at the  $M$ -scheme, which is commonly used in the literature. Also the results in Refs. [155–158], with which we like to compare, are given in this scheme. The  $M$ -scheme is implicitly defined in Ref. [152] and restores the supersymmetric relation

$$\gamma_{qq}^{(n)} + \gamma_{gq}^{(n)} - \gamma_{qg}^{(n)} - \gamma_{gg}^{(n)} = 0 \quad (8.11)$$

between the anomalous dimensions up to 2-loop order. It is not known if this scheme is the same as the  $\overline{\text{MS}}$ -scheme. To proof this the Ward-identities of QCD have to be checked.

The leading order anomalous dimensions do not receive a finite renormalization. At NLO the finite renormalizations between the Larin and the  $M$ -scheme read

$$\gamma_{qq}^{(1),\text{NS},M} = \gamma_{qq}^{(1),\text{NS},L} + 2\beta_0 z_{qq}^{(1)}, \quad (8.12)$$

$$\gamma_{qq}^{(1),\text{PS},M} = \gamma_{qq}^{(1),\text{PS},L}, \quad (8.13)$$

$$\gamma_{qg}^{(1),M} = \gamma_{qg}^{(1),L} + \gamma_{qg}^{(0)} z_{qq}^{(1)}, \quad (8.14)$$

$$\gamma_{gq}^{(1),M} = \gamma_{gq}^{(1),L} - \gamma_{gq}^{(0)} z_{qq}^{(1)}, \quad (8.15)$$

$$\gamma_{gg}^{(1),M} = \gamma_{gg}^{(1),L}. \quad (8.16)$$

The relations at NNLO are given by

$$\gamma_{qq}^{(2),\text{NS},M} = \gamma_{qq}^{(2),\text{NS},L} - 2\beta_0 \left( (z_{qq}^{(1)})^2 - 2z_{qq}^{(2),\text{NS}} \right) + 2\beta_1 z_{qq}^{(1)}, \quad (8.17)$$

$$\gamma_{qq}^{(2),\text{PS},M} = \gamma_{qq}^{(2),\text{PS},L} + 4\beta_0 z_{qq}^{(2),\text{PS}}, \quad (8.18)$$

$$\gamma_{qg}^{(2),M} = \gamma_{qg}^{(2),L} + \gamma_{qg}^{(1),M} z_{qq}^{(1)} + \gamma_{qg}^{(0)} \left( z_{qq}^{(2)} - (z_{qq}^{(1)})^2 \right), \quad (8.19)$$

$$\gamma_{gq}^{(2),M} = \gamma_{gq}^{(2),L} - \gamma_{gq}^{(1),M} z_{qq}^{(1)} - \gamma_{gq}^{(0)} z_{qq}^{(2)}, \quad (8.20)$$

$$\gamma_{gg}^{(2),M} = \gamma_{gg}^{(2),L}, \quad (8.21)$$

with [152]

$$z_{qq}^{(1)} = -\frac{8C_F}{N(N+1)}, \quad (8.22)$$

$$\begin{aligned} z_{qq}^{(2),\text{NS}} &= C_F T_F N_F \frac{16(-3-N+5N^2)}{9N^2(1+N)^2} + C_A C_F \left\{ -\frac{4P_{172}}{9N^3(1+N)^3} - \frac{16}{N(1+N)} S_{-2} \right\} \\ &+ C_F^2 \left\{ \frac{8(2+5N+8N^2+N^3+2N^4)}{N^3(1+N)^3} + \frac{16(1+2N)}{N^2(1+N)^2} S_1 \right. \\ &\left. + \frac{16}{N(1+N)} S_2 + \frac{32}{N(1+N)} S_{-2} \right\}, \end{aligned} \quad (8.23)$$

$$z_{qq}^{(2),\text{PS}} = 8C_F T_F N_F \frac{(N+2)(1+N-N^2)}{N^3(N+1)^3}, \quad (8.24)$$

$$z_{qq}^{(2)} = z_{qq}^{(2),\text{NS}} + z_{qq}^{(2),\text{PS}}. \quad (8.25)$$

These relations can also be found in [158]. Specifically one obtains the following transformations in Mellin- $N$  space:

$$\gamma_{qq}^{(1),\text{NS},M} = \gamma_{qq}^{(1),\text{NS},L} + C_F T_F N_F \frac{64}{3N(N+1)} - C_A C_F \frac{176}{3N(N+1)}, \quad (8.26)$$

## 8. Calculation of Polarized Massive Operator Matrix Elements

$$\gamma_{qq}^{(1),\text{PS},M} = \gamma_{qq}^{(1),\text{PS},L}, \quad (8.27)$$

$$\gamma_{gg}^{(1),M} = \gamma_{gg}^{(1),L} + C_F T_F N_F \frac{64(N-1)}{N^2(N+1)^2}, \quad (8.28)$$

$$\gamma_{gg}^{(1),M} = \gamma_{gg}^{(1),L} - C_F^2 \frac{32(N+2)}{N^2(N+1)^2}, \quad (8.29)$$

$$\gamma_{gg}^{(1),M} = \gamma_{gg}^{(1),L}, \quad (8.30)$$

$$\begin{aligned} \gamma_{qq}^{(2),\text{NS},M} = & \gamma_{qq}^{(2),\text{NS},L} - C_F T_F^2 N_F^2 \frac{256(-3-N+5N^2)}{27N^2(1+N)^2} + C_A C_F T_F N_F \left\{ \frac{64P_{173}}{27N^3(1+N)^3} \right. \\ & \left. + \frac{256}{3N(1+N)} S_{-2} \right\} + C_F^2 T_F N_F \left\{ -\frac{64}{3N^3(1+N)^3} (4+2N \right. \\ & \left. + 5N^2 - 4N^3 + N^4) - \frac{256(1+2N)}{3N^2(1+N)^2} S_1 - \frac{256}{3N(1+N)} S_2 - \frac{512}{3N(1+N)} S_{-2} \right\} \\ & + C_A^2 C_F \left\{ -\frac{16P_{174}}{27N^3(1+N)^3} - \frac{704}{3N(1+N)} S_{-2} \right\} + C_A C_F^2 \left\{ \frac{352(1+N^2)(2+N+2N^2)}{3N^3(1+N)^3} \right. \\ & \left. + \frac{704(1+2N)}{3N^2(1+N)^2} S_1 + \frac{704}{3N(1+N)} S_2 + \frac{1408}{3N(1+N)} S_{-2} \right\}, \end{aligned} \quad (8.31)$$

$$\begin{aligned} \gamma_{qq}^{(2),\text{PS},M} = & \gamma_{qq}^{(2),\text{PS},L} - C_F T_F^2 N_F^2 \frac{128(N+2)(1+N-N^2)}{3N^3(N+1)^3} \\ & + C_A C_F T_F N_F \frac{352(N+2)(1+N-N^2)}{N^3(N+1)^3}, \end{aligned} \quad (8.32)$$

$$\begin{aligned} \gamma_{gg}^{(2),M} = & \gamma_{gg}^{(2),L} - C_F T_F^2 N_F^2 \frac{64(-1+N)(18+21N-17N^2-N^3+10N^4)}{9N^4(1+N)^4} \\ & + C_A C_F T_F N_F \left\{ \frac{32P_{175}}{9N^4(1+N)^4} + \frac{512}{N^2(1+N)^3} S_1 - \frac{128(-1+N)}{N^2(1+N)^2} (S_1^2 + S_2 + S_{-2}) \right\} \\ & + C_F^2 T_F N_F \left\{ \frac{64(-1+N)(2+9N^2+3N^3)}{N^3(1+N)^4} - \frac{128(-1+N)(3+4N)}{N^3(1+N)^3} S_1 \right. \\ & \left. + \frac{128(-1+N)}{N^2(1+N)^2} (S_1^2 - 2S_2 - 2S_{-2}) \right\}, \end{aligned} \quad (8.33)$$

$$\begin{aligned} \hat{\gamma}_{gg}^{(2),M} = & \hat{\gamma}_{gg}^{(2),L} + C_F^2 T_F N_F \left\{ \frac{32(2+N)(6+5N)(3+N-N^2+10N^3)}{9N^4(1+N)^4} \right. \\ & \left. - \frac{256(2+N)}{3N^2(1+N)^2} S_1 \right\}, \end{aligned} \quad (8.34)$$

$$\gamma_{gg}^{(2),M} = \gamma_{gg}^{(2),L}, \quad (8.35)$$

where we introduced the polynomials

$$P_{172} = 36 + 21N + 58N^2 + 140N^3 + 103N^4, \quad (8.36)$$

$$P_{173} = 36 - 12N + 59N^2 + 274N^3 + 203N^4, \quad (8.37)$$

$$P_{174} = 396 + 231N + 944N^2 + 2152N^3 + 1439N^4, \quad (8.38)$$

$$P_{175} = -108 - 237N + 71N^2 - 226N^3 + 73N^4 + 139N^5. \quad (8.39)$$

## 8.2. The Polarized Operator Matrix Element $\Delta A_{qq,Q}^{\text{NS}}$

In this section we present the results for the polarized non-singlet operator matrix element. Although it is known that in the non-singlet case the OMEs and Wilson coefficients have to agree in the polarized and unpolarized case in the  $\overline{\text{MS}}$ -scheme, however, since the renormalization formula contain the constant terms of different OMEs explicitly, cf. Eq. (5.101), we also need the non-singlet OME in the Larin scheme.

### Next-to-Leading Order

At NLO the expression for the unrenormalized non-singlet OME in the Larin-scheme is given by

$$\begin{aligned}
\Delta \hat{A}_{qq,Q}^{\text{NS},(2)} = & C_F T_F \left( \frac{m^2}{\mu^2} \right)^\varepsilon S_\varepsilon^2 \left\{ \frac{1}{\varepsilon^2} \left[ \frac{8(2+3N+3N^2)}{3N(N+1)} - \frac{32}{3} S_1 \right] + \frac{1}{\varepsilon} \left[ -\frac{80}{9} S_1 + \frac{16}{3} S_2 \right. \right. \\
& - \left. \frac{2(12+28N+N^2-6N^3-3N^4)}{9N^2(N+1)^2} \right] + \frac{P_{176}}{54N^3(N+1)^3} - \frac{224}{27} S_1 + \frac{40}{9} S_2 - \frac{8}{3} S_3 \\
& + \left( \frac{2(2+3N+3N^2)}{3N(N+1)} - \frac{8}{3} S_1 \right) \zeta_2 + \varepsilon \left[ -\frac{P_{177}}{648N^4(N+1)^4} - \frac{656}{81} S_1 + \frac{112}{27} S_2 \right. \\
& - \frac{20}{9} S_3 + \frac{4}{3} S_4 - \left. \left( \frac{12+28N+N^2-6N^3-3N^4}{18N^2(N+1)^2} + \frac{20}{9} S_1 - \frac{4}{3} S_2 \right) \zeta_2 \right. \\
& \left. \left. + \left( \frac{2(2+3N+3N^2)}{9N(N+1)} - \frac{8}{9} S_1 \right) \zeta_3 \right] \right\} \quad (8.40)
\end{aligned}$$

with the polynomials

$$P_{176} = 72 + 240N + 344N^2 + 379N^3 + 713N^4 + 657N^5 + 219N^6, \quad (8.41)$$

$$\begin{aligned}
P_{177} = & 432 + 1872N + 3504N^2 + 3280N^3 - 1407N^4 - 7500N^5 \\
& - 9962N^6 - 6204N^7 - 1551N^8. \quad (8.42)
\end{aligned}$$

We can read off the quantities  $a_{qq,Q}^2$  and  $\bar{a}_{qq,Q}^2$  as the  $\varepsilon^0$  and  $\varepsilon^1$  coefficient respectively. These coefficients will be needed for the renormalization of the 3-loop results, cf. Eq. (5.101).

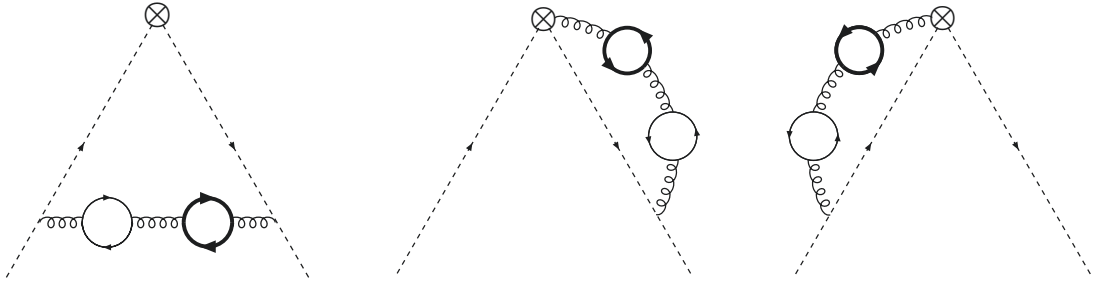


Figure 8.1.: Diagrams contributing to the two-mass corrections of the non-singlet OME.

**Two Mass Contributions**

The two-mass contributions to the NNLO non-singlet OME are given by the graphs in Fig. 8.1. The result reads

$$\begin{aligned}
\Delta \hat{A}_{qq,Q}^{\text{NS,(3)}} = & C_F T_F^2 S_\varepsilon^3 \left\{ \frac{1}{\varepsilon^3} \left[ \frac{512(2+3N+3N^2)}{27N(1+N)} - \frac{2048}{27} S_1 \right] + \frac{1}{\varepsilon^2} \left[ \left( \frac{128(2+3N+3N^2)}{9N(1+N)} \right. \right. \right. \\
& - \left. \left. \frac{512}{9} S_1 \right) (L_1 + L_2) + \frac{128P_{179}}{81N^2(1+N)^2} - \frac{5120}{81} S_1 + \frac{1024}{27} S_2 \right] + \frac{1}{\varepsilon} \left[ \left( \frac{64(2+3N+3N^2)}{3N(1+N)} \right. \right. \\
& - \left. \left. \frac{256}{3} S_1 \right) L_1 L_2 + \left( \frac{32P_{179}}{27N^2(1+N)^2} - \frac{1280}{27} S_1 + \frac{256}{9} S_2 \right) (L_1 + L_2) + \frac{32P_{182}}{81N^3(1+N)^3} \right. \\
& - \frac{256}{81} S_1 (29 + 9H_0^2(\eta)) + \frac{64(2+3N+3N^2)}{9N(1+N)} H_0^2(\eta) + \frac{2560}{81} S_2 - \frac{512}{27} S_3 \\
& + \left( \frac{64(2+3N+3N^2)}{9N(1+N)} - \frac{256}{9} S_1 \right) \zeta_2 \left. \right] + \left( \frac{8(2+3N+3N^2)}{3N(1+N)} - \frac{32}{3} S_1 \right) (L_1^3 + L_2^3) \\
& + \left( \frac{8(2+3N+3N^2)}{3N(1+N)} - \frac{32}{3} S_1 \right) (L_1^2 L_2 + L_1 L_2^2) - 4(L_1^2 + L_2^2) + \left( \frac{8P_{180}}{9N^2(1+N)^2} \right. \\
& - \left. \frac{640}{9} S_1 + \frac{128}{3} S_2 \right) L_1 L_2 + \left( \frac{8P_{182}}{27N^3(1+N)^3} - \frac{1856}{27} S_1 + \frac{640}{27} S_2 - \frac{128}{9} S_3 \right. \\
& + \left. \left( \frac{16(2+3N+3N^2)}{3N(1+N)} - \frac{64}{3} S_1 \right) \zeta_2 \right) (L_1 + L_2) - \frac{10P_{178}}{9\eta N(1+N)} H_0(\eta) - \frac{4P_{183}}{729\eta N^4(1+N)^4} \\
& + \frac{P_{181}}{18\eta N^2(1+N)^2} H_0^2(\eta) - \frac{8(2+3N+3N^2)}{27N(1+N)} H_0^3(\eta) - \frac{16(2+3N+3N^2)}{9N(1+N)} H_0^2(\eta) H_1(\eta) \\
& + \frac{(1+\eta)(5+22\eta+5\eta^2)(2+3N+3N^2)}{36N(1+N)} H_0^2(\eta) \frac{H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})}{\eta^{3/2}} \\
& + \frac{32(2+3N+3N^2)}{9N(1+N)} \left( H_0(\eta) H_{0,1}(\eta) - H_{0,0,1}(\eta) \right) \\
& - \frac{(1+\eta)(5+22\eta+5\eta^2)(2+3N+3N^2)}{9N(1+N)} H_0(\eta) \frac{H_{0,-1}(\sqrt{\eta}) + H_{0,1}(\sqrt{\eta})}{\eta^{3/2}} \\
& + \frac{2(1+\eta)(5+22\eta+5\eta^2)(2+3N+3N^2)}{9N(1+N)} \frac{H_{0,0,-1}(\sqrt{\eta}) + H_{0,0,1}(\sqrt{\eta})}{\eta^{3/2}} \\
& + \left( \frac{16(405-3238\eta+405\eta^2)}{729\eta} - \frac{40(1-\eta^2)}{9\eta} H_0(\eta) + \frac{2(5-78\eta+5\eta^2)}{9\eta} H_0^2(\eta) \right. \\
& + \frac{32}{27} H_0^3(\eta) + \frac{64}{9} H_0^2(\eta) H_1(\eta) - \frac{1}{9} (1+\eta)(5+22\eta+5\eta^2) \frac{H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})}{\eta^{3/2}} H_0^2(\eta) \\
& - \frac{128}{9} H_0(\eta) H_{0,1}(\eta) + \frac{4}{9} (1+\eta)(5+22\eta+5\eta^2) \frac{H_{0,-1}(\sqrt{\eta}) + H_{0,1}(\sqrt{\eta})}{\eta^{3/2}} H_0(\eta) \\
& + \left. \frac{128}{9} H_{0,0,1}(\eta) - \frac{8}{9} (1+\eta)(5+22\eta+5\eta^2) \frac{H_{0,0,-1}(\sqrt{\eta}) + H_{0,0,1}(\sqrt{\eta})}{\eta^{3/2}} \right) S_1 \\
& + \frac{128}{81} S_2 (29 + 9H_0^2(\eta)) - \frac{1280}{81} S_3 + \frac{256}{27} S_4 + \left( \frac{16P_{179}}{27N^2(1+N)^2} - \frac{640}{27} S_1 + \frac{128}{9} S_2 \right) \zeta_2 \\
& + \left. \left( -\frac{64(2+3N+3N^2)}{27N(1+N)} + \frac{256}{27} S_1 \right) \zeta_3 \right\} \tag{8.43}
\end{aligned}$$



with the polynomials

$$P_{178} = 3\eta^2 N^2 + 3\eta^2 N + 2\eta^2 - 3N^2 - 3N - 2, \quad (8.44)$$

$$P_{179} = 3N^4 + 6N^3 - N^2 - 28N - 12, \quad (8.45)$$

$$P_{180} = 15N^4 + 30N^3 + 7N^2 - 56N - 24, \quad (8.46)$$

$$P_{181} = -15\eta^2 N^4 - 30\eta^2 N^3 - 25\eta^2 N^2 - 10\eta^2 N + 18\eta N^4 + 36\eta N^3 - 82\eta N^2 - 356\eta N - 128\eta \\ - 15N^4 - 30N^3 - 25N^2 - 10N, \quad (8.47)$$

$$P_{182} = 135N^6 + 405N^5 + 465N^4 + 271N^3 + 156N^2 + 80N + 24, \quad (8.48)$$

$$P_{183} = 1215\eta^2 N^8 + 4860\eta^2 N^7 + 8100\eta^2 N^6 + 7290\eta^2 N^5 + 3645\eta^2 N^4 + 810\eta^2 N^3 - 1596\eta N^8 \\ - 6384\eta N^7 - 9140\eta N^6 - 756\eta N^5 + 11376\eta N^4 + 14260\eta N^3 + 8496\eta N^2 + 3744\eta N + 864\eta \\ + 1215N^8 + 4860N^7 + 8100N^6 + 7290N^5 + 3645N^4 + 810N^3. \quad (8.49)$$

Using the pole structure in Eq. 5.101 we can extract the  $\mathcal{O}(T_F^2)$  part of the NNLO anomalous dimension  $\gamma_{qq}^{(2),\text{NS}}$  in the Larin-scheme. The explicit expression in the  $M$ -scheme will be given in Section 8.4.

From Eq. 8.43 we can also recover the  $T_F^2$  contributions to the single mass OME by taking the limit  $\eta \rightarrow 1$ . We obtain

$$\Delta a_{qq,Q}^{(3),\text{NS},T_F^2} = C_F T_F^2 \left( \frac{m^2}{\mu^2} \right)^{3\varepsilon/2} S_\varepsilon^3 \left\{ \frac{1}{\varepsilon^3} \left[ -\frac{128(2+3N+3N^2)}{27N(1+N)} + \frac{512}{27} S_1 \right] \right. \\ + \frac{1}{\varepsilon^2} \left[ -\frac{64P_{184}}{81N^2(1+N)^2} + \frac{3584}{81} S_1 - \frac{256}{27} S_2 \right] + \frac{1}{\varepsilon} \left[ -\frac{16P_{185}}{81N^3(1+N)^3} + \frac{4544}{81} S_1 \right. \\ - \frac{1792}{81} S_2 + \frac{128}{27} S_3 + \left. \left( -\frac{16(2+3N+3N^2)}{9N(1+N)} + \frac{64}{9} S_1 \right) \zeta_2 \right] - \frac{4P_{186}}{729N^4(1+N)^4} \\ + \frac{40528}{729} S_1 - \frac{2272}{81} S_2 + \frac{896}{81} S_3 - \frac{64}{27} S_4 + \left( -\frac{8P_{184}}{27N^2(1+N)^2} + \frac{448}{27} S_1 - \frac{32}{9} S_2 \right) \zeta_2 \\ \left. + \left( -\frac{128(2+3N+3N^2)}{27N(1+N)} + \frac{512}{27} S_1 \right) \zeta_3 \right\} \quad (8.50)$$

with the polynomials

$$P_{184} = 33N^4 + 66N^3 + 49N^2 + 4N - 6, \quad (8.51)$$

$$P_{185} = 147N^6 + 441N^5 + 483N^4 + 167N^3 - 18N^2 + 4N + 12, \quad (8.52)$$

$$P_{186} = 4953N^8 + 19812N^7 + 30680N^6 + 21186N^5 + 5787N^4 \\ + 530N^3 + 252N^2 - 288N - 216. \quad (8.53)$$

### 8.3. The Polarized Operator Matrix Element $\Delta A_{gq,Q}$

#### Next-to-Leading Order

The OME  $\Delta A_{gq,Q}^{(2)}$  can be given for general values of  $\varepsilon$  in terms of ratios of  $\Gamma$ -functions. It reads

$$A_{gq,Q}^{(2)} = -16 C_F T_F S_\varepsilon^2 \left( \frac{m^2}{\mu^2} \right)^\varepsilon (N+2) \frac{\Gamma(2-\varepsilon/2)\Gamma(-\varepsilon)\Gamma(\varepsilon/2)\Gamma(N)}{\Gamma(4-\varepsilon)\Gamma(N+2+\varepsilon/2)}. \quad (8.54)$$

Expanding this expression up to the linear term in  $\varepsilon$ , we obtain

$$\begin{aligned} A_{gq,Q}^{(2)} = & C_F T_F (N+2) \left( \frac{m^2}{\mu^2} \right)^\varepsilon S_\varepsilon^2 \left\{ \frac{1}{\varepsilon^2} \frac{32}{3N(N+1)} + \frac{1}{\varepsilon} \left[ \frac{16(2+5N)}{9N(N+1)^2} - \frac{16}{3N(N+1)} S_1 \right] \right. \\ & + \frac{8(22+41N+28N^2)}{27N(N+1)^3} - \frac{8(2+5N)}{9N(N+1)^2} S_1 + \frac{4}{3N(N+1)} S_1^2 + \frac{4}{3N(N+1)} S_2 \\ & + \frac{8}{3N(N+1)} \zeta_2 + \varepsilon \left[ \frac{4(98+369N+408N^2+164N^3)}{81N(N+1)^4} - \left( \frac{4(22+41N+28N^2)}{27N(N+1)^3} \right. \right. \\ & + \left. \left. \frac{2}{3N(N+1)} S_2 \right) S_1 + \frac{2(2+5N)}{9N(N+1)^2} S_1^2 - \frac{2}{9N(N+1)} S_1^3 + \frac{2(2+5N)}{9N(N+1)^2} S_2 \right. \\ & \left. \left. - \frac{4}{9N(N+1)} S_3 + \left( \frac{4(2+5N)}{9N(N+1)^2} - \frac{4}{3N(N+1)} S_1 \right) \zeta_2 + \frac{8}{9N(N+1)} \zeta_3 \right] \right\}. \quad (8.55) \end{aligned}$$

This allows to extract the quantities  $a_{gq,Q}^2$  and  $\bar{a}_{gq,Q}^{(2)}$  from the  $\varepsilon^0$  and  $\varepsilon^1$  part respectively. These will be needed for the renormalization of the 3-loop expressions.

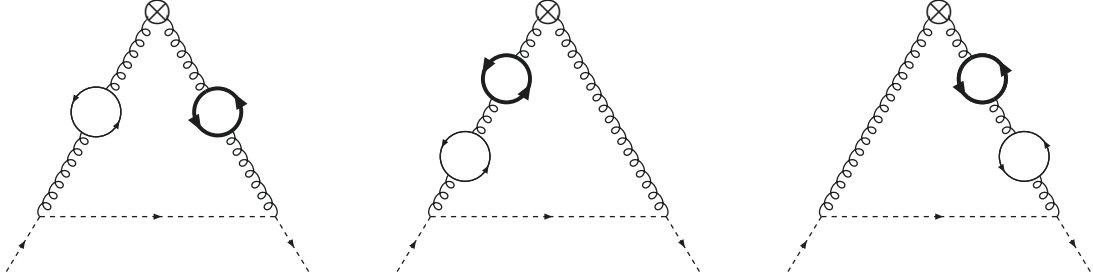


Figure 8.2.: Diagrams contributing to the two-mass corrections to  $\Delta \hat{A}_{gq,Q}$ .

#### Two Mass Contributions

In this Section we want to address the calculation of the two-mass contributions to the polarized OME  $\Delta \hat{A}_{gq,Q}$ , which start at three-loop order. The contributing diagrams are shown in Fig. 8.2. Using the projector given in Eq. (8.10) we find

$$\Delta \hat{A}_{gq,Q} = C_F T_F^2 \left[ 384 \frac{d-6}{d-2} I_{gq,Q}(N) + \frac{1536}{d-2} I_{gq,Q}(N-1) + (m_1 \leftrightarrow m_2) \right], \quad (8.56)$$

where the function  $I_{gq,Q}(N)$  is given by

$$I_{gq,Q}(N) = \left( \frac{4\pi}{\mu} \right)^{3\varepsilon/2} \frac{\Gamma(6-3d/2)\Gamma(N+1)}{\Gamma(N+d/2)} \int_0^1 dz_1 \int_0^1 dz_2 \int_0^1 dz_3 [z_1(1-z_1)]^{1+\varepsilon/2} [z_2(1-z_2)]^{1+\varepsilon/2}$$

$$\times [z_3(1-z_3)]^{-1-\varepsilon/2} \left[ \frac{z_3 m_1^2}{z_1(1-z_1)} + \frac{(1-z_3)m_2^2}{z_2(1-z_2)} \right]^{3\varepsilon/2}. \quad (8.57)$$

We see that the  $N$ -dependence completely factorizes. The integral can be solved using the Mellin-Barnes integral techniques outlined in Chapter 7 before.

We finally obtain

$$\begin{aligned} \Delta \hat{A}_{gq,Q} = & C_F T_F^2 (N+2) S_\varepsilon^3 \left\{ \frac{1024}{9N(N+1)\varepsilon^3} + \frac{1}{\varepsilon^2} \left[ \frac{256}{3N(N+1)} (L_1 + L_2) + \frac{512(2+5N)}{27N(N+1)^2} \right. \right. \\ & - \left. \frac{512}{9N(N+1)} S_1 \right] + \frac{1}{\varepsilon} \left[ \frac{64}{N(N+1)} (L_1^2 + L_2^2) + \left( \frac{128(2+5N)}{9N(1+N)^2} + \frac{64}{N(1+N)} H_0(\eta) \right. \right. \\ & - \left. \left. \frac{128}{3N(1+N)} S_1 \right) L_1 + \left( \frac{128(2+5N)}{9N(1+N)^2} - \frac{64}{N(1+N)} H_0(\eta) - \frac{128}{3N(1+N)} S_1 \right) L_2 \right. \\ & + \frac{128}{3N(1+N)} H_0^2(\eta) + \frac{128(25+48N+29N^2)}{27N(1+N)^3} - \frac{256(2+5N)}{27N(1+N)^2} S_1 + \frac{128}{9N(1+N)} S_1^2 \\ & + \frac{128}{9N(1+N)} S_2 + \frac{128}{3N(1+N)} \zeta_2 \left. \right] + \frac{32}{N(1+N)} (L_1^3 + L_2^3) + \left( \frac{32(2+5N)}{3N(1+N)^2} \right. \\ & + \left. \frac{48}{N(1+N)} H_0(\eta) - \frac{32}{N(1+N)} S_1 \right) L_1^2 + \left( \frac{32(2+5N)}{3N(1+N)^2} - \frac{48}{N(1+N)} H_0(\eta) \right. \\ & - \left. \frac{32}{N(1+N)} S_1 \right) L_2^2 + \left( \frac{32(25+48N+29N^2)}{9N(1+N)^3} + \frac{32(2+5N)}{3N(1+N)^2} H_0(\eta) + \frac{32}{N(1+N)} H_0^2(\eta) \right. \\ & + \left. \left\{ -\frac{64(2+5N)}{9N(1+N)^2} - \frac{32}{N(1+N)} H_0(\eta) \right\} S_1 + \frac{32}{3N(1+N)} S_1^2 + \frac{32}{3N(1+N)} S_2 \right. \\ & + \left. \frac{32}{N(1+N)} \zeta_2 \right) L_1 + \left( \frac{32(25+48N+29N^2)}{9N(1+N)^3} - \frac{32(2+5N)}{3N(1+N)^2} H_0(\eta) + \frac{32}{N(1+N)} H_0^2(\eta) \right. \\ & + \left. \left\{ -\frac{64(2+5N)}{9N(1+N)^2} + \frac{32}{N(1+N)} H_0(\eta) \right\} S_1 + \frac{32}{3N(1+N)} S_1^2 + \frac{32}{3N(1+N)} S_2 \right. \\ & + \left. \frac{32}{N(1+N)} \zeta_2 \right) L_2 + \frac{20(1-\eta^2)}{3\eta N(1+N)} H_0(\eta) - \frac{P_{187}}{3\eta N(1+N)^2} H_0^2(\eta) - \frac{16}{9N(1+N)} H_0^3(\eta) \\ & - \frac{32}{3N(1+N)} H_0^2(\eta) H_1(\eta) + \frac{64}{3N(1+N)} H_0(\eta) H_{0,1}(\eta) - \frac{64}{3N(1+N)} H_{0,0,1}(\eta) \\ & - \frac{8P_{188}}{243\eta N(1+N)^4} + \frac{(1+\eta)(5+22\eta+5\eta^2)}{6\eta^{3/2} N(1+N)} \left[ H_0^2(\eta) \{ H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \} \right. \\ & - \left. 4H_0(\eta) \{ H_{0,-1}(\sqrt{\eta}) + H_{0,1}(\sqrt{\eta}) \} + 8 \{ H_{0,0,-1}(\sqrt{\eta}) + H_{0,0,1}(\sqrt{\eta}) \} \right] \\ & - \left[ \frac{64(25+48N+29N^2)}{27N(1+N)^3} + \frac{64}{3N(1+N)} H_0^2(\eta) + \frac{64}{9N(1+N)} S_2 \right] S_1 + \frac{64(2+5N)}{27N(1+N)^2} S_1^2 \\ & - \frac{64}{27N(1+N)} S_1^3 + \frac{64(2+5N)}{27N(1+N)^2} S_2 - \frac{128}{27N(1+N)} S_3 + \left[ \frac{64(2+5N)}{9N(1+N)^2} \right. \\ & \left. - \frac{64}{3N(1+N)} S_1 \right] \zeta_2 - \frac{128}{9N(1+N)} \zeta_3 \left. \right\}, \quad (8.58) \end{aligned}$$

with the polynomials

$$P_{187} = 5\eta^2 N + 5\eta^2 - 78\eta N - 14\eta + 5N + 5, \quad (8.59)$$

$$P_{188} = 405\eta^2 N^3 + 1215\eta^2 N^2 + 1215\eta^2 N + 405\eta^2 - 3238\eta N^3 - 7626\eta N^2 - 6258\eta N - 1438\eta$$

$$+ 405N^3 + 1215N^2 + 1215N + 405. \quad (8.60)$$

Using the pole prediction in Eq. (5.125) we can extract the  $\mathcal{O}(T_F^2)$  part of the NNLO anomalous dimension  $\gamma_{gg}^{(2)}$ . Since this color factor does not receive a finite renormalization it is directly given in the  $M$ -scheme. The explicit result will be given in Section 8.4.

In the limit  $\eta \rightarrow 1$  we can find the  $\mathcal{O}(T_F^2)$  part of the single mass OME  $\Delta\hat{A}_{gg,Q}$ . For the  $\mathcal{O}(\varepsilon^0)$  part one obtains

$$\begin{aligned} \Delta a_{gg,Q}^{(3),T_F^2} = C_F T_F^2 (N+2) & \left\{ \frac{32(157 + 957N + 1299N^2 + 607N^3)}{243N(N+1)^4} - 64 \left[ \frac{25 + 48N + 29N^2}{27N(N+1)^3} \right. \right. \\ & + \frac{64}{9N(N+1)} S_2 \left. \right] S_1 + \frac{64(2+5N)}{27N(N+1)^2} S_1^2 - \frac{64}{27N(N+1)} S_1^3 + \frac{64(2+5N)}{27N(N+1)^2} S_2 \\ & \left. - \frac{128}{27N(N+1)} S_3 + 64 \left[ \frac{2+5N}{9N(N+1)^2} - \frac{1}{3N(1+N)} S_1 \right] \zeta_2 + \frac{1024}{9N(N+1)} \zeta_3 \right\}. \quad (8.61) \end{aligned}$$

## 8.4. Polarized Anomalous Dimensions from a Massive Calculation

From the 3-loop polarized OMEs one can extract the full NLO splitting functions and the parts  $\mathcal{O}(T_F)$  parts of the NNLO splitting functions, as has been done in Ref. [389] in the unpolarized case. The existence of a single projector in the gluonic, cf. Eq. (8.3), and quarkonic, cf. Eq. (8.10), case respectively is of advantage since the calculational techniques of the unpolarized case had only to be modified slightly. This also applies to the calculation of a series of fixed moments using MATAD [197]. The Feynman diagrams contributing to the massive OMEs were generated by the code QGRAF [362]. The Dirac algebra has been performed using FORM [198, 199] and the color configurations were calculated using the package Color [363] and the Feynman integrals were reduced to master integrals using the integration-by-parts relations [370, 390] implemented in the package Reduze 2 [375, 391]. There are different techniques available to calculate the master integrals, cf. Refs. [347, 367]. For pole terms of the OMEs  $\Delta A_{qq,Q}^{(3),\text{PS}}$ ,  $\Delta A_{Qq}^{(3),\text{PS}}$ ,  $\Delta A_{gg,Q}^{(3)}$ ,  $\Delta A_{gq,Q}^{(3)}$  and  $\Delta A_{gg,Q}^{(3)}$  the contributing master integrals can be calculated by the standard techniques such as the method of hypergeometric functions, the method of hyperlogarithms [392–394], the solution of systems of ordinary differential equation [347, 395–402] and the Almkvist–Zeilberger algorithm [274, 403, 404] since in higher order in the dimensional parameters no elliptic integrals contribute, cf. [281] for a recent survey on these methods. Some of the simpler integrals can be calculated using Mellin–Barnes representations and using the codes [360, 361]. Most of the master integrals were already available from the calculation of the unpolarized three-loop anomalous dimensions in Ref. [389]. Only in a few cases some further differential equations had to be solved to obtain all master integrals. In all the above methods corresponding sum representations have been derived which were solved using the packages Sigma [268, 269], EvaluateMultiSums, SumProduction [271], and HarmonicSums [273, 274]. The constant contributions to the two-loop OMEs  $a_{ij}^{(2)}$  in the Larin scheme are given in [302] for  $a_{Qg}^{(2)}$ , Chapter 4 for  $a_{qq,Q}^{(2),\text{PS}}$ , [405] for  $a_{gg,Q}^{(2)}$  and  $a_{gq,Q}^{(2)}$  can be extracted from Eq. (8.40).

In the following we want to show first results on  $\mathcal{O}(T_F^2)$  and  $\mathcal{O}(T_F)$  contributions to the NNLO splitting functions obtained using the techniques outlined above. This constitutes the first independent check on these parts of the NNLO polarized splitting functions calculated in Ref. [158]. All the following polarized splitting functions are given in the  $M$ -scheme. For the  $\mathcal{O}(T_F^2)$  parts of the anomalous dimensions we obtain

$$\hat{\gamma}_{qq}^{(2),\text{NS}} = C_F T_F^2 \left\{ \frac{8P_{189}}{27N^3(1+N)^3} - \frac{128}{27} S_1 - \frac{640}{27} S_2 + \frac{128}{9} S_3 \right\} \quad (8.62)$$

$$\begin{aligned} \hat{\gamma}_{qq}^{(2),\text{PS}} = & C_F T_F^2 \left\{ -\frac{64(2+N)}{27N^4(N+1)^4} (-9+3N+50N^2+59N^3+7N^4+58N^5) \right. \\ & \left. + \frac{64(2+N)(6+10N-3N^2+11N^3)}{9N^3(N+1)^3} S_1 - \frac{32(N-1)(2+N)}{3N^2(N+1)^2} [S_1^2 + S_2] \right\} \end{aligned} \quad (8.63)$$

$$\begin{aligned} \hat{\gamma}_{qg}^{(2)} = & C_F T_F^2 \left\{ \frac{4P_{191}}{27N^5(1+N)^5} - \left[ \frac{32(-24+4N+47N^2)}{27N^2(N+1)} + \frac{32(N-1)}{3N(1+N)} S_2 \right] S_1 \right. \\ & + \frac{32(N-1)(3+10N)}{9N^2(N+1)} S_1^2 - \frac{32(N-1)}{9N(N+1)} S_1^3 + \frac{32(5N-1)}{3N^2(N+1)} S_2 \\ & \left. + \frac{320(N-1)}{9N(N+1)} S_3 \right\} + C_A T_F^2 \left\{ -\frac{128(1+7N)}{9(1+N)^4} + \frac{16P_{190}}{27N^4(1+N)^3} + \left[ -\frac{32(N-1)}{3N(N+1)} S_2 \right. \right. \\ & \left. + \frac{64(23+50N+10N^2+19N^3)}{27N(N+1)^3} \right] S_1 - \frac{64(-2+5N^2)}{9N(N+1)^2} S_1^2 + \frac{32(N-1)}{9N(N+1)} S_1^3 \\ & - \frac{64(-2+6N+5N^2)}{9N(N+1)^2} S_2 + \frac{64(N-1)}{9N(N+1)} S_3 - \frac{128(5N-2)}{9N(N+1)} S_{-2} + \frac{128(N-1)}{3N(N+1)} S_{-3} \\ & \left. + \frac{128(N-1)}{3N(N+1)} S_{2,1} \right\} \end{aligned} \quad (8.64)$$

$$\begin{aligned} \hat{\gamma}_{gq}^{(2)} = & C_F^2 T_F \left\{ \frac{2P_{196}}{27(N-1)N^5(1+N)^5} + \left[ \frac{32(2+N)P_{193}}{27N^3(1+N)^3} + \frac{208(2+N)}{3N(1+N)} S_2 \right] S_1 \right. \\ & - \frac{16(2+N)(-3+16N+37N^2)}{9N^2(1+N)^2} S_1^2 + \frac{80(2+N)}{9N(1+N)} S_1^3 + \frac{256(2+N)}{9N(1+N)} S_3 \\ & - \frac{16(2+N)(9+46N+67N^2)}{9N^2(1+N)^2} S_2 + \frac{256}{(N-1)N^2(1+N)^2} S_{-2} - \frac{64(2+N)}{3N(1+N)} S_{2,1} \\ & \left. - \frac{128(2+N)}{N(1+N)} \zeta_3 \right\} + C_F C_A T_F \left\{ \frac{8P_{195}}{27(N-1)N^3(1+N)^4} + \left[ -\frac{16P_{194}}{27N^3(1+N)^3} \right. \right. \\ & \left. + \frac{80(2+N)}{3N(1+N)} S_2 \right] S_1 + \frac{16(18+116N+129N^2+43N^3)}{9N^2(1+N)^2} S_1^2 - \frac{80(2+N)}{9N(1+N)} S_1^3 \\ & + \frac{16(-2+16N+9N^2+N^3)}{3N^2(1+N)^2} S_2 + \frac{512(2+N)}{9N(1+N)} S_3 + \left[ -\frac{64P_{192}}{3(N-1)N^2(1+N)^2} \right. \\ & \left. + \frac{256(2+N)}{3N(1+N)} S_1 \right] S_{-2} + \frac{128(2+N)}{3N(1+N)} S_{-3} - \frac{128(2+N)}{3N(1+N)} S_{-2,1} + \frac{128(2+N)}{N(1+N)} \zeta_3 \left\} \right. \\ & \left. + C_F T_F^2 \left\{ \frac{64(2+N)(3+7N+N^2)}{9N(1+N)^3} + \frac{64(2+N)(2+5N)}{9N(1+N)^2} S_1 - \frac{32(2+N)}{3N(1+N)} [S_1^2 + S_2] \right. \right. \\ & \left. + N_F \left\{ \frac{128(2+N)(3+7N+N^2)}{9N(1+N)^3} + \frac{128(2+N)(2+5N)}{9N(1+N)^2} S_1 \right. \right. \\ & \left. \left. - \frac{64(2+N)}{3N(1+N)} [S_1^2 + S_2] \right\} \right\} \end{aligned} \quad (8.65)$$

with the polynomials

$$P_{189} = -24 + 16N + 96N^2 + 35N^3 + 57N^4 + 153N^5 + 51N^6 \quad (8.66)$$

### 8. Calculation of Polarized Massive Operator Matrix Elements

$$P_{190} = 165N^6 + 165N^5 - 488N^4 + 147N^3 - 283N^2 - 162N + 144 \quad (8.67)$$

$$P_{191} = 99N^9 + 297N^8 - 982N^7 - 662N^6 + 1035N^5 - 3079N^4 + 3448N^3 + 2868N^2 \quad (8.68)$$

$$P_{192} = 5N^4 + 9N^3 - 4N^2 - 4N + 6, \quad (8.69)$$

$$P_{193} = 62N^4 - 17N^3 - 76N^2 - 69N - 18, \quad (8.70)$$

$$P_{194} = 418N^5 + 1525N^4 + 1763N^3 + 650N^2 + 444N + 144, \quad (8.71)$$

$$P_{195} = 537N^7 + 1200N^6 - 1013N^5 - 2085N^4 + 1720N^3 - 855N^2 - 2468N - 492, \quad (8.72)$$

$$P_{196} = 1065N^{10} + 6693N^9 + 14084N^8 + 10058N^7 - 3475N^6 - 11707N^5 + 446N^4 + 17132N^3 + 3432N^2 - 6624N - 3456 - 2448N - 1728. \quad (8.73)$$

The non-singlet anomalous dimension is the same in the polarized and unpolarized case. These findings are in full agreement with Ref. [158].<sup>3</sup>

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<sup>3</sup>Note that our differing conventions imply a relative factor of  $-2$  and the replacement  $N_F \rightarrow 2T_F N_F$  between the results given in Ref. [158] and the ones given here.

# 9. Initial State Radiation to $e^+ e^-$ Annihilation Revisited

The next generation collider is most likely an  $e^+ e^-$  collider, like the proposed linear colliders ILC and CLIC [406–408] or circular colliders like the FCC\_ee [409], or even muon colliders [410]. For all these proposed machines the initial state QED corrections (ISR) are of crucial importance for the experimental analyses. This already has been the case for the LEP experiment [411]. In the leading logarithmic series the initial state corrections have been carried out analytically to  $O((\alpha L)^5)$  using the structure function method [412–415] and a small  $z$ -resummation has been performed in [416]. In Ref. [213] the  $O(\alpha^2)$  corrections were calculated neglecting terms of  $\mathcal{O}(\frac{m^2}{s} \ln^2(\frac{m^2}{s}))$ . Here  $s$  is the centre-of-mass energy squared and  $m = m_e$  is the electron mass. These corrections are used in analysis codes such as TOPAZO [417] and ZFITTER [418, 419] used to determine the precision observables like the  $Z$ -mass and width from LEP data. In Ref. [214] this calculation was done using the factorization into massless cross section and massive operator matrix elements in the asymptotic limit. The logarithmic terms of these two calculations agree. However, the constant parts deviate significantly from each other.

This discrepancy triggered our interest. The only way to find the origin of this mismatch consists in calculating the scattering cross section without any approximation and performing the expansion in  $m^2/s \ll 1$  at the end along with a highly precise numerical control. In this chapter we will present the results of this calculation. It has the following structure. First, we will present the Born cross section and the factorization into massless cross section and massive operator matrix element. In Section 9.2 we review the  $\mathcal{O}(\alpha)$  initial state corrections including the full mass dependence. Afterwards, in Section 9.3, we turn to the  $\mathcal{O}(\alpha^2)$  initial state corrections. First, the corrections due to fermion pair production are presented. We split them up into the various production mechanisms (the non-singlet, the pure singlet and their interference contribution) following Ref. [213]. We also discuss discrepancies in the literature and show their numerical impact on the radiator function. In the last section the correction due to photon emissions are addressed. We will present the corrections due to soft and virtual photon emission, the hard emission is still work in progress and will not be presented here. Further details on the calculation are given in Appendix E.

## 9.1. The Born Cross Section and Factorization

The Born cross section is given by the process

$$e^-(p_-) + e^+(p_+) \rightarrow V(q) \rightarrow f^-(q_-) + f^+(q_+) \quad (9.1)$$

and its differential and integrated cross sections are given by, cf. Ref. [420],

$$\begin{aligned} \frac{d\sigma^{(0)}}{d\Omega} &= \frac{\alpha^2}{4s} \sqrt{1 - \frac{4m_f^2}{s}} \left[ \left( 1 + \cos^2(\theta) + \frac{4m_f^2}{s} \sin^2(\theta) \right) G_1(s) \right. \\ &\quad \left. - \frac{8m_f^2}{s} G_2(s) + 2\sqrt{1 - \frac{4m_f^2}{s}} \cos(\theta) G_3(s) \right] \end{aligned} \quad (9.2)$$

## 9. Initial State Radiation to $e^+e^-$ Annihilation Revisited

$$\sigma^{(0)}(s) = \frac{4\pi\alpha^2}{3s} \sqrt{1 - \frac{4m_f^2}{s}} \left[ \left(1 + \frac{2m_f^2}{s}\right) G_1(s) - \frac{6m_f^2}{s} G_2(s) \right] \quad (9.3)$$

In this formula  $\alpha$  denotes the fine structure constant,  $m_f$  the mass of the colorless final state fermion,  $\Omega$  is the spherical angle and  $\theta$  the scattering angle in the center-of-mass system of the collision. The effective couplings read

$$G_1(s) = Q_e^2 Q_f^2 + 2Q_e Q_f v_e v_f \text{Re} [\chi_Z(s)] + (v_e^2 + a_e^2)(v_f^2 + a_f^2) |\chi_Z(s)|^2, \quad (9.4)$$

$$G_2(s) = (v_e^2 + a_e^2) a_f^2 |\chi_Z(s)|^2, \quad (9.5)$$

$$G_3(s) = 2Q_e Q_f a_e a_f \text{Re} [\xi_Z(s)] + 4v_e v_f a_e a_f |\chi_Z(s)|^2, \quad (9.6)$$

where the reduced  $Z$ -propagator is given by

$$\chi_Z(s) = \frac{s}{s - M_Z^2 + iM_Z\Gamma_Z}. \quad (9.7)$$

$M_Z$  and  $\Gamma_Z$  denote the mass and width of the  $Z$ -boson respectively and  $Q_{e(f)}$  is the electromagnetic charges of the electron (final state fermion). The electroweak vector  $v_i$  and axial  $a_i$  couplings can be expressed through the electroweak mixing angle  $\theta_w$  and the third component of the weak isospin of the respective particle  $I_{w,i}^3 = \pm\frac{1}{2}$  via

$$v_{e(f)} = \frac{1}{\sin(\theta_w) \cos(\theta_w)} \left[ I_{w,e(f)}^3 - 2Q_e \sin^2(\theta_w) \right], \quad (9.8)$$

$$a_{e(f)} = \frac{1}{\sin(\theta_w) \cos(\theta_w)} I_{w,e(f)}^3. \quad (9.9)$$

These relations are important in global fits of the electroweak parameters since they can reduce the number of independent ones.

At the first order of QED one has also effects of virtual gauge bosons and an additional photon can be radiated from the initial state

$$e^-(p_-) + e^+(p_+) \rightarrow V(q) + \gamma(k). \quad (9.10)$$

The vector boson  $V$  subsequently decays further.

At the next order up to two loop virtual photonic corrections can contribute. Furthermore, two photons

$$e^-(p_-) + e^+(p_+) \rightarrow V(q) + \gamma(k_1) + \gamma(k_2) \quad (9.11)$$

or a fermion pair

$$e^-(p_-) + e^+(p_+) \rightarrow V(q) + f^-(k_-) + f^+(k_+) \quad (9.12)$$

can be radiated into the final state.

Since we only consider initial state radiation, the cross section factorizes according to the Drell-Yan process developed in the context of QCD. One derives radiator functions to the Born process via [213]

$$\frac{d\sigma}{ds'} = \sigma(s') \frac{1}{4s} \sum_{n=0}^{\infty} \int d^4q \delta(q^2 - s') \frac{1}{(2\pi)^{3n}} \prod_{i=1}^n d^4k_i \delta(k_i^2 - m_i^2) \theta(k_i^0) \delta^4(p_- + p_+ - q - K) |T^{(n)}|^2. \quad (9.13)$$



Here  $K$  is the sum of all momenta of additionally emitted particles and  $|T^{(n)}|^2$  denotes the matrix element of the process with  $n$  additional particles in the final state. Here and in the following we will use the invariants

$$\begin{aligned} s &= (p_- + p_+)^2, & s' &= q^2 = (q_- + q_+)^2 \\ s'' &= (k_+ + k_-)^2 \quad \text{or} \quad (k_1 + k_2)^2 \end{aligned} \quad (9.14)$$

It is also convenient to introduce the dimensionless quantities

$$z = \frac{s'}{m^2}, \quad \rho = \frac{m^2}{s}, \quad \beta = \sqrt{1 - \frac{4m^2}{s}}. \quad (9.15)$$

We will also use

$$L = \ln \left( \frac{s}{m^2} \right). \quad (9.16)$$

Schematically this can also be written as

$$\frac{d\sigma_{e^+e^-}}{ds'} = \frac{1}{s} \sigma_{e^+e^-}(s') H \left( z, \alpha, \frac{s}{m^2} \right), \quad (9.17)$$

where the radiator function  $H(z, \alpha, \frac{s}{m^2})$  obeys the following expansion

$$H \left( z, \alpha, \frac{s}{m^2} \right) = \delta(1-z) + \sum_{k=1}^{\infty} \left( \frac{\alpha}{4\pi} \right)^k C_k \left( z, \frac{s}{m^2} \right) \quad (9.18)$$

$$C_k \left( z, \frac{s}{m^2} \right) = \sum_{l=0}^k \ln^{k-l} \left( \frac{s}{m^2} \right) c_{k,l}(z), \quad (9.19)$$

In Ref. [213] the calculation of QED initial state radiation neglecting power suppressed terms in the mass has been achieved. The authors also used the factorization in the asymptotic limit, i.e.  $s \gg m^2$ , to compute the logarithmic terms using renormalization group techniques and operator matrix elements. In Ref. [214] this calculation has been extended to the constant terms and therefore exhausted the reach of the asymptotic limit. In the asymptotic limit the cross section factorizes into, cf. Ref. [214],

$$\begin{aligned} \frac{d\sigma}{ds'} &= \frac{\sigma^{(0)}}{s} \otimes \left[ \Gamma_{e^+e^+} \left( \frac{\mu^2}{m_e^2} \right) \otimes \tilde{\sigma}_{e^+e^-} \left( \frac{\mu^2}{m_e^2} \right) \otimes \Gamma_{e^-e^-} \left( \frac{s'}{\mu^2} \right) \right. \\ &+ \Gamma_{\gamma e^+} \left( \frac{\mu^2}{m_e^2} \right) \otimes \tilde{\sigma}_{e^- \gamma} \left( \frac{\mu^2}{m_e^2} \right) \otimes \Gamma_{e^-e^-} \left( \frac{s'}{\mu^2} \right) \\ &+ \Gamma_{e^+e^+} \left( \frac{\mu^2}{m_e^2} \right) \otimes \tilde{\sigma}_{e^+ \gamma} \left( \frac{\mu^2}{m_e^2} \right) \otimes \Gamma_{e^- \gamma} \left( \frac{s'}{\mu^2} \right) \\ &\left. + \Gamma_{e^+ \gamma} \left( \frac{\mu^2}{m_e^2} \right) \otimes \tilde{\sigma}_{\gamma \gamma} \left( \frac{\mu^2}{m_e^2} \right) \otimes \Gamma_{e^- \gamma} \left( \frac{s'}{\mu^2} \right) \right]. \end{aligned} \quad (9.20)$$

The process in the last line does not contribute to  $\mathcal{O}(\alpha^2)$ . The  $\tilde{\sigma}_{ij}$  are the massless scattering cross sections and the  $\Gamma_{ij}$  are the process independent massive operator matrix elements of local twist-2 operators, completely in analogy to the case of QCD discussed in the chapters before. The Feynman rules have to be slightly adjusted to recover the Abelian case, cf. Ref. [214], and the external electrons have to be taken massive. The results of the constant part, however, were found to disagree between the two calculations. As a first step to understand the mismatch we recomputed the OMEs for

process II and III and found agreement with the calculation of Ref. [214], except of two misprints which we want to correct here. In Eq. (147) of Ref. [214]  $\text{Li}_2(1-x)$  should be multiplied by 2 and Eq. (170) should read

$$\begin{aligned} \bar{\Gamma}_{\gamma e}^{(0)} \otimes P_{e\gamma}^{(0)}(z) = & -\frac{16}{3}(1+z)\ln^3(z) - 8\left(3 + \frac{4}{3z} + 2z\right)\ln^2(z) - 4\left(16 + \frac{76}{9z} + 14z\right. \\ & \left. + (1+z)\zeta_2\right)\ln(z) - 2(20 + \zeta_2)(1-z) - \frac{8}{3}\left(\frac{128}{9} + \zeta_2\right)\frac{1-z^3}{z}. \end{aligned} \quad (9.21)$$

Note also the following misprints in Refs. [213, 421], which are relevant for this chapter. In Eq. (2.42) of Ref. [213] compared to [422–424]  $\frac{16}{9}z$  should read  $\frac{16}{9z}$ . The last term in Eq. (B.11) [421] should read  $(47 - 100z)$ . These errors are not mentioned in Ref. [425] and neither in the Erratum to [421]. They have been corrected in the Drell-Yan code by W.L. van Neerven, however, the term given in [426] is correct.

## 9.2. The $\mathcal{O}(\alpha)$ Corrections

The first radiative correction to  $e^+ e^-$  annihilation is given by the process where an additional photon is radiated off the initial state electron or positron

$$e^+ + e^- \rightarrow \gamma^*/Z^* + \gamma \quad (9.22)$$

and associated virtual corrections. The cross section can be decomposed into three parts

$$\frac{d\sigma^{(1),I}}{ds'} = \frac{d\sigma^{(0)}}{s} \left(\frac{\alpha}{\pi}\right) \left[ \delta(1-z) \left( \delta_1^{S1}(\lambda, \varepsilon) + \delta_1^{V1}(\lambda) \right) + \theta(1-z-\varepsilon) \delta_1^{H1}(z) \right]. \quad (9.23)$$

Here  $\lambda$  is a photon mass introduced to regulate collinear divergencies of the massless photons and  $\varepsilon$  is the soft-hard separator for the real photon. It is defined by demanding

$$k^0 > \frac{\sqrt{s\varepsilon}}{2} \quad (9.24)$$

for hard photons. In the full cross section the dependencies on  $\varepsilon$  and  $\lambda$  have to drop out. These regulators allows us to calculate in  $d = 4$  dimensions. We can therefore deal with the  $\gamma_5$  problem without a finite renormalization. This is only possible since we work in pure QED. The non-Abelian nature of QCD makes an analogous treatment far more involved. The corrections  $\delta_1^{H1}(z)$  and  $\delta_1^{S1}(\varepsilon, \lambda)$  are the contributions of the diagrams in Fig. 9.2 for hard and soft photon momentum respectively. The contribution  $\delta_1^{V1}(\lambda)$  is due to the virtual corrections induced by the diagrams in Fig. 9.3.

At this order it is easily possible to derive the full mass dependence of these three parts. After the integration over the two particle phase space given in Appendix E.2 the hard photon contribution is

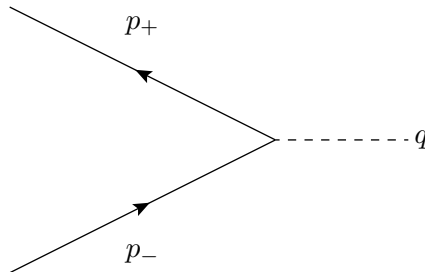


Figure 9.1.: The diagrams contributing to the Born cross section of the process  $e^+ + e^- \rightarrow \gamma^*/Z^*$ .

given by

$$\begin{aligned} \delta_1^{H_1}(z) &= -\frac{1}{(1+x)^2(1-z)} \left[ 1 + z^2 + x^2(1+z^2) + 2x(3+z^2) \right] - \frac{1}{(1-x)(1+x)^3(1-z)} \\ &\times \left[ 1 + z^2 + x^4(1+z^2) + 4x(2-z+z^2) + 4x^3(2-z+z^2) + 2x^2(3-4z+3z^2) \right] \ln(x) \\ &= \frac{1+z}{1-z} [L-1] + \mathcal{O}\left(\frac{m^2}{s}\right). \end{aligned} \quad (9.25)$$

The limit of small electron mass,  $\rho = m^2/s \ll 1$  reproduces the result given in Ref. [213, 214]. To compactify the resulting expression we have introduced the variable

$$x = \frac{1-\beta}{1+\beta}. \quad (9.26)$$

This allows to express the arguments of the occurring functions in a simple manner.

The virtual corrections can be extracted from the one-loop form factor  $F^{(1)}(s)$ . In general, since we consider the full mass dependence, we also have to consider the form factor  $F^{(2)}(s)$  which is always power suppressed in the ratio  $\rho$ . However, at  $\mathcal{O}(\alpha)$  only  $F^{(1)}(s)$  contributes. Using the results in Refs. [427, 428] we find

$$\begin{aligned} \delta_1^{V_1}(\lambda) &= 2 \left( 1 + \frac{2m^2}{s} \right) \text{Re} \left( F^{(1)}(s) \right) \\ &= \frac{1+4x+x^2}{(1+x)^3} \left\{ -2(1+x) - (1+x) \ln\left(\frac{\lambda^2}{m^2}\right) + \frac{2x}{2(1-x)} \ln(x) \right. \\ &\quad \left. - \frac{1+x^2}{1-x} \left[ \frac{1}{2} \ln^2(x) + \frac{3}{2} \ln(x) - 2 \ln(1-x) \ln(x) + \ln\left(\frac{\lambda^2}{m^2}\right) \ln(x) + 2\text{Li}_2(x) - 4\zeta_2 \right] \right\} \\ &= \left[ -\frac{1}{2}L^2 + \ln\left(\frac{\lambda^2}{m^2}\right)L + \frac{3}{2}L - \ln\left(\frac{\lambda^2}{m^2}\right) - 2 + 4\zeta_2 \right] + \mathcal{O}\left(\frac{m^2}{s}\right). \end{aligned} \quad (9.27)$$

Since in Ref. [213] the goal was only the asymptotic representation, the kinematic factor  $1 + 2m^2/s$  was set to unity from the start.

The last building block are the soft contributions. In the soft limit the amplitude factorizes

$$k \rightarrow 0 : \quad \left| T^{(1)}(k, q) \right|^2 = S(k) \left| T^{(0)}(q) \right|^2, \quad (9.28)$$

with  $|T^{(0)}|^2$  the Born amplitude given by the graph in Fig. 9.1 and  $S(k)$  the soft-photon approximation of the amplitude where a single photon is emitted into the final state, cf. [429]

$$S(k) = \left( \frac{p_+^\mu}{k \cdot p_+} - \frac{p_-^\mu}{k \cdot p_-} \right)^2. \quad (9.29)$$



Figure 9.2.: Diagrams contributing to the  $\mathcal{O}(\alpha)$  radiative contribution due to real radiation.

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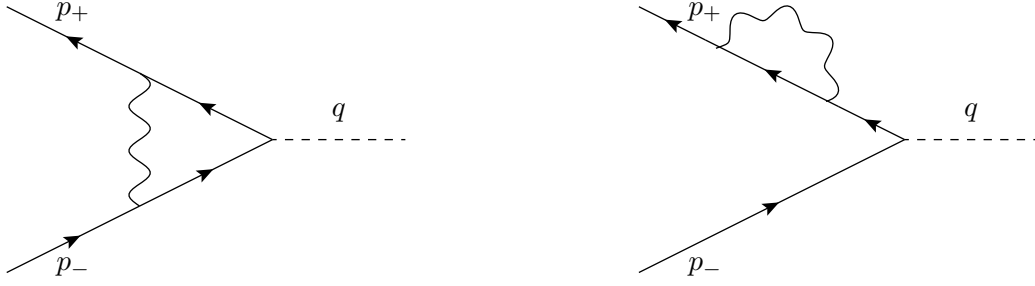


Figure 9.3.: Diagrams contributing to the  $\mathcal{O}(\alpha)$  corrections due to virtual photons.

The soft term is therefore given by the integral

$$\frac{d\sigma^{(1),S_1}}{ds'} = \frac{\sigma^{(0)}}{4s} \frac{1}{(2\pi)^3} \int d^4q \int d^4k \delta(q^2 - s') \delta(k^2) \delta^{(4)}(p_+ + p_- - q - k) |T^{(1)}(k, q)|^2 \quad (9.30)$$

$$\rightarrow \frac{\sigma^{(0)}}{4s} \frac{1}{(2\pi)^3} \int d^4q \delta(q^2 - s') \delta^{(4)}(p_+ + p_- - q) |T^{(0)}(q)|^2 \int d^4k \delta(k^2) S(k). \quad (9.31)$$

Performing the phase space integrations we arrive at

$$\begin{aligned} \delta_1^{S_1}(\lambda, \varepsilon) &= \frac{1 + 4x + x^2}{(1+x)^3} \left\{ -2(1+x) \ln(1+x) - 2(1+x) \ln(\varepsilon) + (1+x) \ln\left(\frac{\lambda^2}{m^2}\right) \right. \\ &\quad - \frac{2x(1+x)}{1-x} \ln(x) + \frac{1+x^2}{1-x} \left[ \frac{1}{2} \ln^2(x) - 2 \ln(\varepsilon) \ln(x) + 2 \ln(1-x) \ln(x) \right. \\ &\quad \left. \left. - 2 \ln(1+x) \ln(x) + \ln\left(\frac{\lambda^2}{m^2}\right) \ln(x) + 2\text{Li}_2(x) - 2\zeta_2 \right] \right\} \\ &= -\frac{1}{2} L^2 - \ln\left(\frac{\lambda^2}{m^2}\right) L + 2 \ln(\varepsilon) L + \ln\left(\frac{\lambda^2}{m^2}\right) - 2 \ln(\varepsilon) - 2z_2 + \mathcal{O}\left(\frac{m^2}{s}\right). \end{aligned} \quad (9.32)$$

Putting all contributions together we arrive at the complete first order correction

$$\begin{aligned} \frac{d\sigma^{(1),I}}{ds'} &= \frac{d\sigma^{(0)}}{s} \frac{\alpha}{\pi} \left[ \delta(1-z) \left\{ -\frac{1}{(1+x)^2(1-z)} \left[ 1 + z^2 + x^2(1+z^2) + 2x(3+z^2) \right] \right. \right. \\ &\quad - \frac{1}{(1-x)(1+x)^3(1-z)} \left[ 1 + z^2 + x^4(1+z^2) + 4x(2-z+z^2) + 4x^3(2-z+z^2) \right. \\ &\quad \left. \left. + 2x^2(3-4z+3z^2) \right] \ln(x) \right\} \\ &\quad + \theta(1-z-\varepsilon) \frac{1+4x+x^2}{(1+x)^3} \left\{ -2(1+x) \left( 1 + \ln(1+x) + \ln(\varepsilon) \right) - \frac{2x(1+2x)}{1-x} \ln(x) \right. \\ &\quad \left. + \frac{1+x^2}{1-x} \left( 4 \ln(1-x) \ln(x) - 2 \ln(1+x) \ln(x) - 2 \ln(\varepsilon) \ln(x) + 4\text{Li}_2(x) \right) \right\} \right] \\ &= \frac{d\sigma^{(0)}}{s} \frac{\alpha}{\pi} \left[ \delta(1-z) \left( -2 + \frac{3}{2} L + 2\zeta_2 + 2(L-1) \ln(\varepsilon) \right) \right. \\ &\quad \left. + \theta(1-z-\varepsilon) \frac{1+z^2}{1-z} (L-1) \right] + \mathcal{O}\left(\frac{m^2}{s}\right). \end{aligned} \quad (9.33)$$

## 9.3. The $\mathcal{O}(\alpha^2)$ Corrections

### 9.3.1. Corrections due to Electron Pair Production

A new class of corrections, which emerge at  $\mathcal{O}(\alpha^2)$ , are the corrections due the emission of an electron-positron pair radiated off the initial state. Since these corrections start at  $\mathcal{O}(\alpha^2)$  they do not receive virtual contributions. Furthermore, because all initial and final state particles are massive, the cross sections are finite without introducing regulatory masses or UV-cutoffs. This section will deal with the calculation of these corrections. They can be grouped into four categories based on the production mechanism of the electron-positron pair. The non-singlet contribution, called process II in Ref. [213], the pure-singlet contribution (process III), their interference (process IV) and additionally further processes not discussed in Ref. [213] but included in the full calculations for the massless Drell-Yan cross sections, cf. Ref. [421]. In the end we will discuss differences with the results of Ref. [213] and show their numerical impact on the radiator function.

#### Process II

The graphs corresponding to process II (the non-singlet contribution) are shown in Fig. 9.4. Due to the fact that the fermion pair in the final state completely factorizes from the phase space parametrization, it is possible to find a very compact one-dimensional integral representation for this contribution, cf. [430, 431]. This representation can be achieved by explicit factorization of the phase space or by using the general parametrization of the phase space derived in Appendix E and integrating out the angles and one of the invariants. However, care has to be taken when neglecting the electron mass. Denoting the mass of the initial state fermions with  $m_i$  and the one of the final state fermions with  $m_f$  the general formula for the non-singlet cross section reads

$$\begin{aligned} \frac{d\sigma^{(2),\text{II}}(z, m_i, m_f)}{ds'} = & \frac{\sigma^0(s')}{s} a^2 \int_{4m_f^2}^{s(1-\sqrt{z})^2} ds'' \frac{16}{3s s''^2} \sqrt{1 - \frac{4m_f^2}{s''} (2m_f^2 + s'')} \left\{ \right. \\ & - \frac{\lambda^{1/2}(s, s', s'') [2s s' s'' + m_i^2 (s^2 + (s' - s'')^2) + 4s m_i^4]}{s s' s'' + m_i^2 (s^2 + (s' - s'')^2 - 2s (s' + s''))} \\ & \left. + \frac{(s' + s'')^2 + 4m_i^2 (s - s' - s'') + s^2 - 8m_i^4}{\beta(s - s' - s'')} \ln \left( \frac{s - s' - s'' + \beta \lambda^{1/2}(s, s', s'')}{s - s' - s'' - \beta \lambda^{1/2}(s, s', s'')} \right) \right\} \end{aligned} \quad (9.34)$$

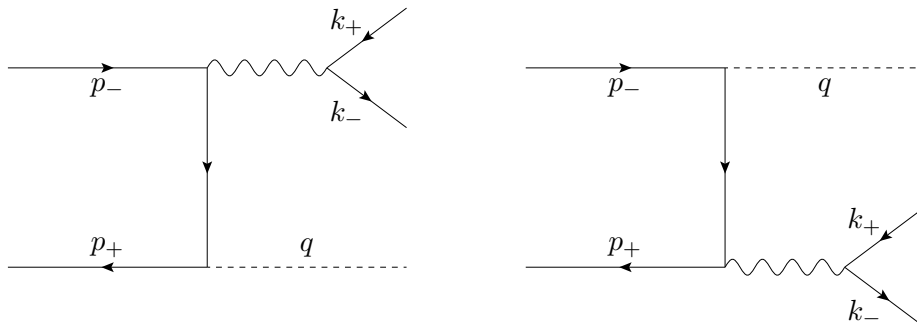


Figure 9.4.: The graphs contributing to process II, the non-singlet contribution.

## 9. Initial State Radiation to $e^+ e^-$ Annihilation Revisited

with  $\beta = \sqrt{1 - 4m_i^2/s}$ . This formula has been validated with both phase space parametrizations mentioned above.

Neglecting initial state masses,  $m_i \rightarrow 0$ , we obtain

$$\begin{aligned} \frac{d\sigma^{(2),\text{II}}(z, 0, m_f = m)}{ds'} &= \frac{\sigma^{(0)}(s')}{s} a^2 \int_{4m^2}^{s(1-\sqrt{z})^2} ds'' \frac{16}{3s s''^2} \sqrt{1 - \frac{4m^2}{s''}} (2m^2 + s'') \left\{ \right. \\ &\quad \left. - 2\lambda^{1/2}(s, s', s'') + \frac{s^2 + (s' + s'')^2}{s - s' - s''} \ln \left( \frac{s - s' - s'' + \lambda^{1/2}(s, s', s'')}{s - s' - s'' - \lambda^{1/2}(s, s', s'')} \right) \right\} \quad (9.35) \end{aligned}$$

and reproduce the formula given in Refs. [213, 431]. However, this approximation is only valid, if the final state fermions are *heavy* with respect to the initial state fermions. This is the case, for example, when considering  $\mu^+ \mu^-$  production. In the case of initial state radiation, where we consider electrons in the initial and final state, this approximation is not valid. This can be seen most conveniently by introducing the new variable

$$y = \frac{4m^2}{s''}. \quad (9.36)$$

The difference, already expanded in the electron mass, then reads

$$\begin{aligned} \delta\Pi &= \frac{d\sigma^{(2),\text{II}}(z, m, m)}{ds'} - \frac{d\sigma^{(2),\text{II}}(z, 0, m)}{ds'} \\ &= \frac{\sigma^{(0)}(s')}{s} a^2 \int_0^1 dy \frac{8}{3y} \sqrt{1-y}(2+y) \left\{ \frac{(1-z)(1-(4-z)z)y}{4z + (1-z)^2y} \right. \\ &\quad \left. + \frac{1+z^2}{1-z} \ln \left( \frac{4z}{4z + (1-z)^2y} \right) \right\} + \mathcal{O} \left( \frac{m^2}{s} L^2 \right) \\ &= \frac{\sigma^{(0)}(s')}{s} a^2 \left\{ -\frac{128}{9} \left[ 3 + \frac{1}{(1-z)^3} - \frac{2}{(1-z)^2} - 2z \right] - 16 \left[ 1 + \frac{5z}{3} + \frac{8}{9} \frac{1}{(1-z)^4} \right. \right. \\ &\quad \left. \left. - \frac{20}{9} \frac{1}{(1-z)^3} + \frac{4}{9} \frac{1}{(1-z)^2} \right] \ln(z) + \frac{8}{3} \frac{1+z^2}{1-z} \left[ \frac{10}{9} - \frac{14}{3} \ln(z) - \ln^2(z) \right] \right\} + \mathcal{O} \left( \frac{m^2}{s} L^2 \right). \quad (9.37) \end{aligned}$$

To compute the expanded result, the integrand and the integration boundaries have been expanded in  $\rho$  simultaneously. This is in general not possible, since expansion and integration do not commute. However, since the final expression of the difference has a Taylor expansion around  $\rho = 0$  this is possible in this case. We checked that higher terms in the expansion of the integrand as well as the integration boundary only contribute power suppressed terms in the final result.

The closed form solution of the full integral in Eq. (9.34) for  $m_i = m_f = m$  in terms of iterated integrals is given by

$$\begin{aligned} \frac{d\sigma^{(2),\text{II}}(z, \rho)}{ds'} &= \frac{\sigma^{(0)}(s')}{s} a^2 \left\{ \frac{64}{3} z(1-z)(1+z-4\rho) \tilde{\text{H}}_{v_4, d_7} + \frac{256}{3} z\rho(1+z-4\rho) \tilde{\text{H}}_{v_4, d_6} \right. \\ &\quad + \frac{128z(1-4\rho^2)(1-z+2\rho)(1-z-4\rho)}{3(1-z)^2} \tilde{\text{H}}_{d_8, d_7} \\ &\quad \left. + \frac{512z\rho(1-4\rho^2)(1-z+2\rho)(1-z-4\rho)}{3(1-z)^3} \tilde{\text{H}}_{d_8, d_6} \right\} \end{aligned}$$

$$\begin{aligned}
 & + \frac{16}{9(1-z)^2} \left[ (1+z)^2(4-9z+4z^2) + 2(9-16z+13z^2-2z^3)\rho + 32\rho^2 \right] \tilde{\text{H}}_{d_2} \\
 & + \frac{512z\rho}{9(1-z)^4} \left[ 3(1-z)^4z - (1-z)^3(4+z^2)\rho - 2(9-29z+38z^2-17z^3+3z^4)\rho^2 \right. \\
 & - 4(2-z)(3+6z-5z^2)\rho^3 + 16(7-8z+9z^2)\rho^4 + 128(3-z)\rho^5 \left. \right] \tilde{\text{H}}_{d_4} \\
 & - \frac{16}{9(1-z)^4} \left[ 3-34z+129z^2-212z^3+129z^4-34z^5+3z^6+8(2-16z+9z^2 \right. \\
 & + 4z^3-5z^4+2z^5)\rho + 16z(12-13z+18z^2-z^3)\rho^2 + 32(1+22z-7z^2)\rho^3 \left. \right] \tilde{\text{H}}_{d_1} \\
 & - \frac{128z}{9(1-z)^4} \left[ 1+7z-47z^2+86z^3-47z^4+7z^5+z^6-2(7-55z+54z^2 \right. \\
 & + 16z^3-17z^4+3z^5)\rho - 4(39-16z+16z^2+4z^3+5z^4)\rho^2 \\
 & + 16(8-23z+22z^2+9z^3)\rho^3 + 128(7+2z-z^2)\rho^4 \left. \right] \tilde{\text{H}}_{d_5} - \frac{64}{3}(2z+(1-z)\rho)\tilde{\text{H}}_{d_3} \\
 & + \left[ \frac{16}{3\sqrt{1-4\rho}}(1+z-4\rho)\tilde{\text{H}}_{v_4} + \frac{32(1-4\rho^2)(1-z+2\rho)(1-z-4\rho)}{3(1-z)^3\sqrt{1-4\rho}}\tilde{\text{H}}_{d_8} \right] \\
 & \times \ln \left( \frac{1-z-4\rho-\sqrt{1-4\rho}\sqrt{(1-z)^2-8(1+z)\rho+16\rho^2}}{1-z-4\rho+\sqrt{1-4\rho}\sqrt{(1-z)^2-8(1+z)\rho+16\rho^2}} \right) \left. \right\} \quad (9.38)
 \end{aligned}$$

This result has been achieved using the same techniques used to find the closed form solution of the pure-singlet contribution to DIS at NLO discussed in Chapter 3.3. We introduce a modified iterated integral  $\tilde{\text{H}}$  to accomodate the massive phase space. It is also defined iteratively

$$\tilde{\text{H}}_{w_1, \dots, w_n}(x) = \int_x^1 dt w_1 \tilde{\text{H}}_{w_1, \dots, w_{n-1}}(t). \quad (9.39)$$

In this chapter we use the abbreviations

$$\tilde{\text{H}}_{w_1, \dots, w_n} \left( \frac{4\rho}{(1-\sqrt{x})^2} \right) \equiv \tilde{\text{H}}_{w_1, \dots, w_n}, \quad \text{H}_{w_1, \dots, w_n}(r) \equiv \text{H}_{w_1, \dots, w_n}, \quad (9.40)$$

to suppress the arguments of the iterated integrals. The letters are given by

$$d_1 = \frac{1}{\sqrt{1-t}\sqrt{16\rho^2-8\rho(1+z)t+(1-z)^2t^2}}, \quad (9.41)$$

$$d_2 = \frac{t}{\sqrt{1-t}\sqrt{16\rho^2-8\rho(1+z)t+(1-z)^2t^2}}, \quad (9.42)$$

$$d_3 = \frac{1}{t\sqrt{1-t}\sqrt{16\rho^2-8\rho(1+z)t+(1-z)^2t^2}}, \quad (9.43)$$

$$d_4 = \frac{1}{(16\rho^2+(4z-8\rho(1+z))t+(1-z)^2t^2)\sqrt{1-t}\sqrt{16\rho^2-8\rho(1+z)t+(1-z)^2t^2}}, \quad (9.44)$$

$$d_5 = \frac{t}{(16\rho^2+(4z-8\rho(1+z))t+(1-z)^2t^2)\sqrt{1-t}\sqrt{16\rho^2-8\rho(1+z)t+(1-z)^2t^2}}, \quad (9.45)$$

$$d_6 = \frac{1}{(16\rho^2+(4z-8\rho(1+z))t+(1-z)^2t^2)\sqrt{16\rho^2-8\rho(1+z)t+(1-z)^2t^2}}, \quad (9.46)$$

$$d_7 = \frac{t}{(16\rho^2+(4z-8\rho(1+z))t+(1-z)^2t^2)\sqrt{16\rho^2-8\rho(1+z)t+(1-z)^2t^2}}, \quad (9.47)$$

$$d_8 = \frac{1-z}{(4\rho - (1-z)t)\sqrt{1-t}}, \quad (9.48)$$

$$d_9 = \frac{1}{(16\rho^2 + 4(z - 2\rho(1+z))t + (1-z)^2 t^2)\sqrt{1-t}} \quad (9.49)$$

$$d_{10} = \frac{t}{(16\rho^2 + 4(z - 2\rho(1+z))t + (1-z)^2 t^2)\sqrt{1-t}} \quad (9.50)$$

$$d_{11} = \frac{1}{t\sqrt{16\rho^2 - 8\rho(1+z)t + (1-z)^2 t^2}} \quad (9.51)$$

$$d_{12} = \frac{1}{16\rho^2 + 4(z - 2\rho(1+z))t + (1-z)^2 t^2} \quad (9.52)$$

$$d_{13} = \frac{t}{16\rho^2 + 4(z - 2\rho(1+z))t + (1-z)^2 t^2} \quad (9.53)$$

$$v_1 = \frac{1}{\sqrt{1-4t}\sqrt{16t^2 - 8(1+z)t + (1-z)^2}} \quad (9.54)$$

$$v_2 = \frac{1}{t\sqrt{1-4t}\sqrt{16t^2 - 8(1+z)t + (1-z)^2}} \quad (9.55)$$

$$v_3 = \frac{1}{\sqrt{1-4t}(4t - (1+z))\sqrt{16t^2 - 8(1+z)t + (1-z)^2}}, \quad (9.56)$$

$$v_4 = \frac{1}{t\sqrt{1-t}}, \quad (9.57)$$

The limit  $\rho \rightarrow 0$  is not easily computed. Our way to approach the integrals in this limit is based on two steps. First we expand the integrand around  $\rho = 0$  up to the constant contribution. This term will serve as a subtraction term. This integral is easily evaluated in the original phase space, but after integration one recognises that the result does not match the numerical expectation. The second step is to transform the difference of the original and the subtraction term into the integration variable

$$t = \frac{1}{1 - \left(1 - \frac{1-\sqrt{z}}{4\rho}\right)w}, \quad (9.58)$$

with the integration over  $w \in (0, 1)$ . After this transformation the difference does not vanish in the limit  $\rho \rightarrow 0$  and the second contribution to the integral can be computed. The sum of both contribution agrees with the numerical integration of (9.38) for small values of  $\rho$ . We finally find

$$\begin{aligned} \frac{d\sigma^{(2),\text{II}}(z, \rho)}{ds'} &= \frac{\sigma^{(0)}(s')}{s} \left(\frac{\alpha}{4\pi}\right)^2 \left\{ \frac{8}{3} \frac{1+z^2}{1-z} L^2 - \left[ \frac{16}{9} \frac{11-12z+11z^2}{1-z} + \frac{16}{3} \frac{1+z^2}{1-z} H_0 \right. \right. \\ &+ \left. \left. \frac{32}{3} \frac{1+z^2}{1-z} H_1 \right] L + \frac{32}{9(1-z)^3} (7-13z+8z^2-13z^3+7z^4) - \frac{16z}{9(1-z)^4} (3-36z \right. \\ &+ \left. 94z^2-72z^3+19z^4) H_0 - \frac{8z^2}{3(1-z)} H_0^2 + \left( \frac{32}{9} \frac{11-12z+11z^2}{1-z} + \frac{16}{3} \frac{2+z^2}{1-z} H_0 \right) H_1 \right. \\ &\left. + \frac{32}{3} \frac{1+z^2}{1-z} H_1^2 + \frac{16z^2}{3(1-z)} H_{0,1} - \frac{16(2+3z^2)}{3(1-z)} \zeta_2 \right\} + \mathcal{O}\left(\frac{m^2}{s} L^2\right). \quad (9.59) \end{aligned}$$

This result differs from the one presented in Ref. [213] exactly by the term given in Eq. (9.37) and agrees with the result obtained in Ref. [214] based on massive operator matrix elements.



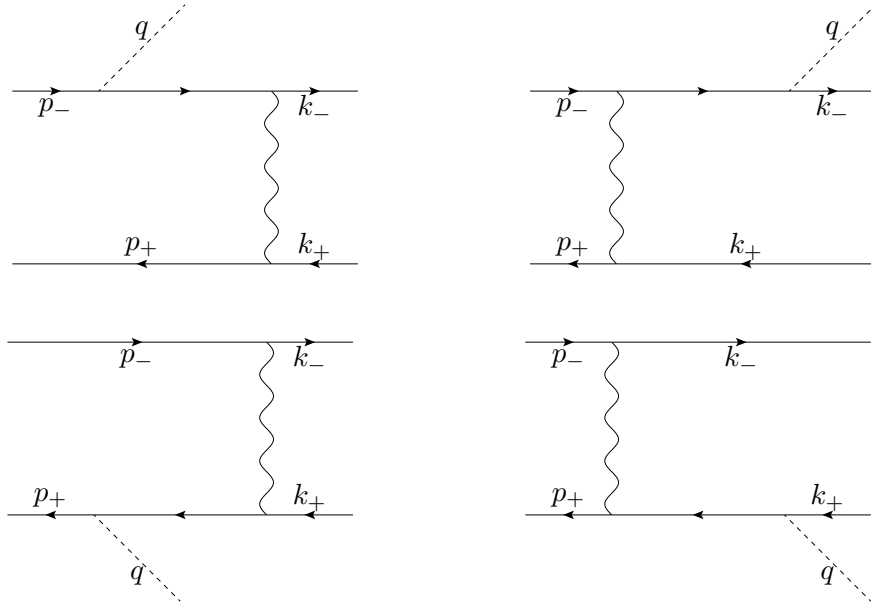


Figure 9.5.: The graphs contributing to process III, the pure-singlet contribution.

### Process III

The pure-singlet contributions are given by the diagrams in Fig. 9.5. Following the procedure in Refs. [422, 423], we split process III into two contributions. The first comes only from the diagrams in one column of Fig. 9.5 and will be called *squared* contribution. The other one is the interference between the graphs from both columns. The interference contribution was already found to be regularization scheme independent and regular in the limit  $\rho \rightarrow 0$ , cf. Refs. [422, 423]. Therefore we can expand the integrand and perform the phase space integral to obtain the contribution in this limit in a straight forward manner. We obtain

$$\begin{aligned}
 \frac{d\sigma_{\text{interf}}^{(2),\text{III}}}{ds'} &= \frac{\sigma^{(0)}(s')}{s} \left(\frac{\alpha}{4\pi}\right)^2 \left\{ -160(1-z) - \left[ 16(5+4z) - 80(1+z)H_{-1} + \frac{48(2+2z+z^2)}{z}H_{-1}^2 \right] H_0 \right. \\
 &- \left[ 52z - \frac{40(2+2z+z^2)}{z}H_{-1} \right] H_0^2 - \frac{16}{3}zH_0^3 + \left[ 8(5-4z)H_0 - \frac{8(4-6z+3z^2)}{z}H_0^2 \right] H_1 \\
 &- \frac{4(4-6z+3z^2)}{z}H_0H_1^2 - \left[ 8(5-4z) - \frac{8(8-2z+5z^2)}{z}H_0 - \frac{8(4-6z+3z^2)}{z}H_1 \right] H_{0,1} \\
 &- \left[ 80(1+z) + \frac{32(5+2z^2)}{z}H_0 - \frac{96(2+2z+z^2)}{z}H_{-1} \right] H_{0,-1} - \frac{32(2+2z+z^2)}{z}H_{0,0,1} \\
 &+ \frac{16(10-10z+3z^2)}{z}H_{0,0,-1} - \frac{8(4-6z+3z^2)}{z}H_{0,1,1} - \frac{96(2+2z+z^2)}{z}H_{0,-1,-1} \\
 &+ \left. \left[ 8(10+z) + 160H_0 - \frac{8(4-6z+3z^2)}{z}H_1 - \frac{48(2+2z+z^2)}{z}H_{-1} \right] \zeta_2 + 32(5+z)\zeta_3 \right\} \\
 &+ \mathcal{O}\left(\frac{m^2}{s}\right) \equiv \left(\frac{\alpha}{4\pi}\right)^2 \delta_{\text{interf}}^{\text{PS}} \tag{9.60}
 \end{aligned}$$

in full agreement with Refs. [421–423] after adjusting the color factors to obtain the abelian limit.<sup>1</sup> Since this contribution is unquestioned in the limit  $\rho \rightarrow 0$  we did not derive its full mass dependence

<sup>1</sup>One has to set  $C_F = T_F = 1$  and  $C_A = 0$ .

in terms of iterated integrals.

The contributions from the squared diagrams contain mass logarithms. Therefore this contributions cannot be compared with [422, 423], since this calculation concerned massless quarks. The quark mass was only introduced as a regulator and neglected whenever possible. As we have seen for process II already, this is not allowed when the fully massive cross section shall be computed. The angular integrals can be computed using the list in Appendix E.2, afterwards the integration over the first invariant can be done using standard techniques. The integration over the last invariant  $s''$  can be achieved using the same technique as for process II an the pure-singlet contributions to DIS. The result for the full mass dependence in terms of iterated integrals reads

$$\begin{aligned}
 \frac{d\sigma_{\text{square}}^{(2),\text{III}}}{ds'} &= \frac{\sigma^{(0)}(s')}{s} \left(\frac{\alpha}{4\pi}\right)^2 \left\{ -\frac{32S_1(1-\sqrt{z})^2 z P_{197}}{1-4\rho} \left[ 4\tilde{\text{H}}_{d_6} + \frac{1-z}{\rho} \tilde{\text{H}}_{d_7} \right] + 512P_{198}\tilde{\text{H}}_{d_{12},d_3} \right. \\
 &+ 2048zP_{198}\tilde{\text{H}}_{d_{12},d_4} - \frac{128(1+z)P_{198}}{\rho} \tilde{\text{H}}_{d_{12},d_1} + \frac{512z(1+z-8\rho)P_{198}}{\rho} \tilde{\text{H}}_{d_{12},d_5} \\
 &+ \frac{32zP_{199}}{\rho} \left[ 4\tilde{\text{H}}_{v_4,d_6} + \frac{1-z}{\rho} \tilde{\text{H}}_{v_4,d_7} \right] + \frac{64(1-z)P_{200}}{3\rho^2} \tilde{\text{H}}_{d_{11},d_{10}} \\
 &+ \frac{128(z-2\rho)P_{200}}{3\rho^2} \tilde{\text{H}}_{d_{11},d_9} + \frac{16P_{201}}{3\rho^2} \tilde{\text{H}}_{d_3} + \frac{32(1-\sqrt{z})(1-z)zP_{202}}{\rho(1-4\rho)} \left[ 4\tilde{\text{H}}_{d_{10},d_6} + \frac{1-z}{\rho} \tilde{\text{H}}_{d_{10},d_7} \right] \\
 &- \frac{64(1-\sqrt{z})(1-z)^2 z P_{203}}{3\rho^2(1-4\rho)(z-4\rho)} \tilde{\text{H}}_{d_7,d_{10}} - \frac{128(1-\sqrt{z})(1-z)z(z-2\rho)P_{203}}{3\rho^2(1-4\rho)(z-4\rho)} \tilde{\text{H}}_{d_7,d_9} \\
 &+ \frac{128zP_{204}}{\rho(1-4\rho)} \left[ 4\tilde{\text{H}}_{d_9,d_6} + \frac{1-z}{\rho} \tilde{\text{H}}_{d_9,d_7} \right] + \frac{256(1-z)zP_{205}}{3\rho^2(1-4\rho)(z-4\rho)} \tilde{\text{H}}_{d_6,d_{10}} \\
 &+ \frac{512z(z-2\rho)P_{205}}{3\rho^2(1-4\rho)(z-4\rho)} \tilde{\text{H}}_{d_6,d_9} - \frac{2(1-z)^2 P_{206}}{3\rho^2(1-4\rho)^2(1+z-4\rho)^2(z-4\rho)} \tilde{\text{H}}_{d_2} \\
 &+ \frac{8P_{207}}{3\rho^2(1-4\rho)^2(1+z-4\rho)^2(z-4\rho)} \tilde{\text{H}}_{d_1} - \frac{16zP_{208}}{3\rho^2(1-4\rho)^2(1+z-4\rho)^2(z-4\rho)} \tilde{\text{H}}_{d_5} \\
 &- \frac{64zP_{209}}{3\rho^2(1-4\rho)^2(1+z-4\rho)^2(z-4\rho)} \tilde{\text{H}}_{d_4} - \frac{32(1+z)(z+\rho)}{\rho} \tilde{\text{H}}_{0,d_1} + 128(z+\rho)\tilde{\text{H}}_{0,d_3} \\
 &+ 512z(z+\rho)\tilde{\text{H}}_{0,d_4} + \frac{128z(z+\rho)(1+z-8\rho)}{\rho} \tilde{\text{H}}_{0,d_5} \\
 &+ \frac{16(1-z)(1+z)(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_1,d_{10}} + \frac{32(1+z)(z-2\rho)(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_1,d_9} \\
 &+ \frac{16(1-z)(1+z)(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_{10},d_1} - \frac{64(1-z)\rho(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_{10},d_3} \\
 &- \frac{256(1-z)z\rho(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_{10},d_4} - \frac{64(1-z)z(1+z-8\rho)(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_{10},d_5} \\
 &+ \frac{32(1-z)^2(1+z)(z+\rho)}{\rho} \tilde{\text{H}}_{d_{13},d_1} - 128(1-z)^2(z+\rho)\tilde{\text{H}}_{d_{13},d_3} \\
 &- 512(1-z)^2z(z+\rho)\tilde{\text{H}}_{d_{13},d_4} - \frac{128(1-z)^2z(z+\rho)(1+z-8\rho)}{\rho} \tilde{\text{H}}_{d_{13},d_5} \\
 &- \frac{64(1-z)\rho(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_3,d_{10}} - \frac{128\rho(z-2\rho)(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_3,d_9} \\
 &- \frac{256(1-z)z\rho(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_4,d_{10}} - \frac{512z\rho(z-2\rho)(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_4,d_9} \\
 &- \frac{64(1-z)z(1+z-8\rho)(1+5z+4\rho)}{S_1} \tilde{\text{H}}_{d_5,d_{10}}
 \end{aligned}$$

$$\begin{aligned}
 & - \frac{128z(1+z-8\rho)(z-2\rho)(1+5z+4\rho)}{S_1} \tilde{H}_{d_5, d_9} \\
 & + \frac{32(1+z)(z-2\rho)(1+5z+4\rho)}{S_1} \tilde{H}_{d_9, d_1} - \frac{128\rho(z-2\rho)(1+5z+4\rho)}{S_1} \tilde{H}_{d_9, d_3} \\
 & - \frac{512z\rho(z-2\rho)(1+5z+4\rho)}{S_1} \tilde{H}_{d_9, d_4} - \frac{128z(1+z-8\rho)(z-2\rho)(1+5z+4\rho)}{S_1} \tilde{H}_{d_9, d_5} \\
 & + 2048z(1+z)^2 \rho^2 \tilde{H}_{d_{11}, d_1, d_6} + 512(1-z)z(1+z)^2 \rho \tilde{H}_{d_{11}, d_1, d_7} \\
 & - 8192z(1+z) \rho^3 \tilde{H}_{d_{11}, d_3, d_6} - 2048(1-z)z(1+z) \rho^2 \tilde{H}_{d_{11}, d_3, d_7} \\
 & - 32768z^2(1+z) \rho^3 \tilde{H}_{d_{11}, d_4, d_6} - 8192(1-z)z^2(1+z) \rho^2 \tilde{H}_{d_{11}, d_4, d_7} \\
 & - 8192z^2(1+z) \rho^2(1+z-8\rho) \tilde{H}_{d_{11}, d_5, d_6} - 2048(1-z)z^2(1+z) \rho(1+z-8\rho) \tilde{H}_{d_{11}, d_5, d_7} \\
 & + 2048z(1+z)^2 \rho^2 \tilde{H}_{d_{11}, d_6, d_1} - 8192z(1+z) \rho^3 \tilde{H}_{d_{11}, d_6, d_3} \\
 & - 32768z^2(1+z) \rho^3 \tilde{H}_{d_{11}, d_6, d_4} - 8192z^2(1+z) \rho^2(1+z-8\rho) \tilde{H}_{d_{11}, d_6, d_5} \\
 & + 512(1-z)z(1+z)^2 \rho \tilde{H}_{d_{11}, d_7, d_1} - 2048(1-z)z(1+z) \rho^2 \tilde{H}_{d_{11}, d_7, d_3} \\
 & - 8192(1-z)z^2(1+z) \rho^2 \tilde{H}_{d_{11}, d_7, d_4} - 2048(1-z)z^2(1+z) \rho(1+z-8\rho) \tilde{H}_{d_{11}, d_7, d_5} \\
 & - 32(1-z)(1+z)(1+z+\rho) \tilde{H}_{v_4, d_1, d_{10}} - 64(1+z)(1+z+\rho)(z-2\rho) \tilde{H}_{v_4, d_1, d_9} \\
 & - 32(1-z)(1+z)(1+z+\rho) \tilde{H}_{v_4, d_{10}, d_1} + 128(1-z)\rho(1+z+\rho) \tilde{H}_{v_4, d_{10}, d_3} \\
 & + 512(1-z)z\rho(1+z+\rho) \tilde{H}_{v_4, d_{10}, d_4} + 128(1-z)z(1+z-8\rho)(1+z+\rho) \tilde{H}_{v_4, d_{10}, d_5} \\
 & + 128(1-z)\rho(1+z+\rho) \tilde{H}_{v_4, d_3, d_{10}} + 256\rho(1+z+\rho)(z-2\rho) \tilde{H}_{v_4, d_3, d_9} \\
 & + 512(1-z)z\rho(1+z+\rho) \tilde{H}_{v_4, d_4, d_{10}} + 1024z\rho(1+z+\rho)(z-2\rho) \tilde{H}_{v_4, d_4, d_9} \\
 & + 128(1-z)z(1+z-8\rho)(1+z+\rho) \tilde{H}_{v_4, d_5, d_{10}} + 256z(1+z+\rho)(z-2\rho)(1+z-8\rho) \tilde{H}_{v_4, d_5, d_9} \\
 & - 64(1+z)(1+z+\rho)(z-2\rho) \tilde{H}_{v_4, d_9, d_1} + 256\rho(1+z+\rho)(z-2\rho) \tilde{H}_{v_4, d_9, d_3} \\
 & + 1024z\rho(1+z+\rho)(z-2\rho) \tilde{H}_{v_4, d_9, d_4} + 256z(1+z+\rho)(z-2\rho)(1+z-8\rho) \tilde{H}_{v_4, d_9, d_5} \\
 & + \frac{1}{\sqrt{1-4\rho}} \left[ \frac{32S(1-\sqrt{z})^2 P_{197}}{\rho(1-4\rho)} - \frac{32P_{199}}{\rho^2} \tilde{H}_{v_4} - \frac{128P_{204}}{\rho^2(1-4\rho)} \tilde{H}_{d_9} \right. \\
 & - \frac{32(1-\sqrt{z})(1-z)P_{202}}{\rho^2(1-4\rho)} \tilde{H}_{d_{10}} - 512(1+z)^2 \rho \tilde{H}_{d_{11}, d_1} + 2048(1+z) \rho^2 \tilde{H}_{d_{11}, d_3} \\
 & \left. + 8192z(1+z) \rho^2 \tilde{H}_{d_{11}, d_4} + 2048z(1+z) \rho(1+z-8\rho) \tilde{H}_{d_{11}, d_5} \right] H_{v_1} \\
 & + \frac{1}{\sqrt{1-4\rho}} \left[ -\frac{8S_1(1-\sqrt{z})^3(1+\sqrt{z})P_{197}}{\rho(1-4\rho)} + \frac{8(1-z)P_{199}}{\rho^2} \tilde{H}_{v_4} + \frac{32(1-z)P_{204}}{\rho^2(1-4\rho)} \tilde{H}_{d_9} \right. \\
 & + \frac{8(1-\sqrt{z})(1-z)^2 P_{202}}{\rho^2(1-4\rho)} \tilde{H}_{d_{10}} + 128(1-z)(1+z)^2 \rho \tilde{H}_{d_{11}, d_1} - 512(1-z)(1+z) \rho^2 \tilde{H}_{d_{11}, d_3} \\
 & \left. - 2048(1-z)z(1+z) \rho^2 \tilde{H}_{d_{11}, d_4} - 512(1-z)z(1+z) \rho(1+z-8\rho) \tilde{H}_{d_{11}, d_5} \right] H_{v_2} \\
 & + \frac{1}{\sqrt{1-4\rho}} \left[ \frac{128S(1-\sqrt{z})^2 z P_{197}}{\rho(1-4\rho)} - \frac{128zP_{199}}{\rho^2} \tilde{H}_{v_4} - \frac{512zP_{204}}{\rho^2(1-4\rho)} \tilde{H}_{d_9} \right. \\
 & - \frac{128(1-\sqrt{z})(1-z)zP_{202}}{\rho^2(1-4\rho)} \tilde{H}_{d_{10}} - 2048z(1+z)^2 \rho \tilde{H}_{d_{11}, d_1} + 8192z(1+z) \rho^2 \tilde{H}_{d_{11}, d_3} \\
 & \left. + 32768z^2(1+z) \rho^2 \tilde{H}_{d_{11}, d_4} - 8192z^2(1+z) \rho(-1-z+8\rho) \tilde{H}_{d_{11}, d_5} \right] H_{v_3}
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{\sqrt{1-4\rho}} \left[ \frac{16S(1-\sqrt{z})^2 P_{197}}{\rho(1-4\rho)} - \frac{16P_{199}}{\rho^2} \tilde{H}_{v_4} - \frac{64P_{204}}{\rho^2(1-4\rho)} \tilde{H}_{d_9} \right. \\
 & - \frac{16(1-\sqrt{z})(1-z)P_{202}}{\rho^2(1-4\rho)} \tilde{H}_{d_{10}} - 256(1+z)^2 \rho \tilde{H}_{d_{11},d_1} + 1024(1+z)\rho^2 \tilde{H}_{d_{11},d_3} \\
 & \left. + 4096z(1+z)\rho^2 \tilde{H}_{d_{11},d_4} + 1024z(1+z)\rho(1+z-8\rho) \tilde{H}_{d_{11},d_5} \right] \ln \left( \frac{1-z}{1+z} \right), \quad (9.61)
 \end{aligned}$$

with the polynomials

$$P_{197} = 12\rho^2 + \rho(2z + 2\sqrt{z} - 7) - 3z, \quad (9.62)$$

$$P_{198} = -z^2 + \rho^2(3z + 1) + \rho(2z + 1)z, \quad (9.63)$$

$$P_{199} = 2\rho^3 - 3z^2 + \rho^2(1 - 3z) + \rho z(z + 4), \quad (9.64)$$

$$P_{200} = 32\rho^4 - 32\rho^3 + \rho^2(13z^2 + 48z + 8) + 10z^2 - \rho z(31z + 12), \quad (9.65)$$

$$P_{201} = 36\rho^4 + \rho^2(-6z^2 + 12z + 4) + 2z^2 + 2\rho^3(6z - 18\sqrt{z} - 61) - \rho z(z + 36), \quad (9.66)$$

$$\begin{aligned}
 P_{202} = & -8\rho^3 \left( z^{3/2} - z - 2\sqrt{z} - 4 \right) - \rho z \left( 13z^{3/2} + 13z + 4\sqrt{z} + 4 \right) \\
 & + 2\rho^2 \left( 2z^{5/2} + 14z^{3/2} + 2z^2 + 6z + \sqrt{z} - 3 \right) + 3 \left( z^{5/2} + z^2 \right) - 32\rho^4 (\sqrt{z} + 1), \quad (9.67)
 \end{aligned}$$

$$\begin{aligned}
 P_{203} = & -\rho z \left( 61z^{3/2} + 61z + 42\sqrt{z} + 42 \right) - 4\rho^3 \left( 84z^{3/2} + 6z^2 + 114z + 29\sqrt{z} + 41 \right) \\
 & + \rho^2 \left( 73z^{5/2} + 261z^{3/2} + 97z^2 + 273z + 20\sqrt{z} + 20 \right) \\
 & + 10 \left( z^{5/2} + z^2 \right) + 32\rho^4 (3z + 7\sqrt{z} + 10), \quad (9.68)
 \end{aligned}$$

$$\begin{aligned}
 P_{204} = & +8\rho^4 \left( 2z^{3/2} + z^2 - z + 2\sqrt{z} - 4 \right) + \rho^2 z \left( 8z^{3/2} + 24z^2 + 57z + 4\sqrt{z} + 3 \right) \\
 & - 2\rho^3 \left( 4z^{5/2} + 12z^{3/2} + 2z^3 + 36z^2 + 3z + 4\sqrt{z} - 3 \right) + 32\rho^5 (z + 1) \\
 & + 3z^3 - \rho z^2 (19z + 10), \quad (9.69)
 \end{aligned}$$

$$\begin{aligned}
 P_{205} = & 32\rho^5 \left( 3z^{3/2} + 26z + 3\sqrt{z} + 26 \right) - 10z^3 - \rho^2 z (198z^2 + 503z + 98) + \rho z^2 (81z + 62) \\
 & - 4\rho^4 \left( 6z^{5/2} + 30z^{3/2} + 180z^2 + 447z + 12\sqrt{z} + 103 \right) \\
 & + \rho^3 \left( 24z^{5/2} + 12z^{3/2} + 125z^3 + 1202z^2 + 795z + 52 \right), \quad (9.70)
 \end{aligned}$$

$$\begin{aligned}
 P_{206} = & 22528\rho^7 + 128\rho^5 (3z^2 + 50z + 198) + 18z^2 (z + 1)^2 + 32\rho^4 (19z^3 + 346z^2 + 102z - 208) \\
 & - 8\rho^3 (10z^4 + 512z^3 + 1191z^2 + 328z - 103) - \rho z (161z^3 + 504z^2 + 381z + 38) \\
 & + \rho^2 (400z^4 + 2414z^3 + 2908z^2 + 550z - 40) - 512\rho^6 (23z + 84), \quad (9.71)
 \end{aligned}$$

$$\begin{aligned}
 P_{207} = & -20(z-1)z^2(z+1)^2 - 1024\rho^7 \left( 18z^{3/2} + 7z^2 - 72z + 18\sqrt{z} - 19 \right) \\
 & - 256\rho^6 \left( -54z^{5/2} - 126z^{3/2} + 3z^3 + 254z^2 + 115z - 72\sqrt{z} - 78 \right) \\
 & + 64\rho^5 \left( -54z^{7/2} - 234z^{5/2} - 288z^{3/2} + 11z^4 + 481z^3 + 859z^2 - 563z - 108\sqrt{z} - 236 \right) \\
 & - 16\rho^4 \left( -18z^{9/2} - 162z^{7/2} - 360z^{5/2} - 288z^{3/2} + 5z^5 + 421z^4 + 2080z^3 + 257z^2 - 1919z \right. \\
 & \left. - 72\sqrt{z} - 256 \right) + 4\rho^3 \left( -36z^{9/2} - 162z^{7/2} - 234z^{5/2} - 126z^{3/2} + 136z^5 + 1899z^4 \right. \\
 & \left. + 2880z^3 - 2088z^2 - 2364z - 18\sqrt{z} - 127 \right) + 2\rho z \left( 96z^4 + 213z^3 - 59z^2 - 213z - 37 \right) \\
 & + \rho^2 \left( 18z^{9/2} + 54z^{7/2} + 54z^{5/2} + 18z^{3/2} - 585z^5 - 2864z^4 - 1126z^3 + 3128z^2 + 1343z + 24 \right) \\
 & + 8192\rho^8 (2z - 7), \quad (9.72)
 \end{aligned}$$

$$\begin{aligned}
 P_{208} = & -2z^2(z+1)^2(9z^2+2z-11) + 2048\rho^7 \left( -126z^{3/2} + 60z^2 + 185z - 162\sqrt{z} + 99 \right) \\
 & - 1024\rho^6 \left( -81z^{5/2} - 243z^{3/2} + 56z^3 + 196z^2 + 222z - 144\sqrt{z} + 16 \right) \\
 & + 128\rho^5 \left( -90z^{7/2} - 522z^{5/2} - 720z^{3/2} + 116z^4 + 648z^3 + 767z^2 + 95z - 252\sqrt{z} - 202 \right) \\
 & - 32\rho^4 \left( -18z^{9/2} - 234z^{7/2} - 612z^{5/2} - 504z^{3/2} + 66z^5 + 885z^4 + 1472z^3 - 21z^2 - 964z \right. \\
 & \left. - 108\sqrt{z} - 314 \right) + 8\rho^3 \left( -36z^{9/2} - 198z^{7/2} - 306z^{5/2} - 162z^{3/2} + 16z^6 + 670z^5 \right. \\
 & \left. + 2174z^4 + 1091z^3 - 1837z^2 - 1465z - 18\sqrt{z} - 185 \right) + 2\rho^2 \left( 18z^{9/2} + 54z^{7/2} \right. \\
 & \left. + 54z^{5/2} + 18z^{3/2} - 192z^6 - 1441z^5 - 2152z^4 + 490z^3 + 2304z^2 + 871z + 40 \right) \\
 & + \rho z \left( 157z^5 + 580z^4 + 394z^3 - 484z^2 - 551z - 96 \right) - 16384\rho^8 \left( 7z - 18\sqrt{z} + 17 \right), \quad (9.73)
 \end{aligned}$$

$$\begin{aligned}
 P_{209} = & 65536\rho^9 + 2z^3(z+1)^2 + 1024\rho^7 \left( 27z^{3/2} + 62z^2 + 29z + 36\sqrt{z} - 100 \right) \\
 & + \rho z^2 \left( z^3 - 40z^2 - 67z - 26 \right) + \rho^2 z \left( -123z^4 - 151z^3 + 411z^2 + 503z + 96 \right) \\
 & - 128\rho^6 \left( 54z^{5/2} + 180z^{3/2} + 164z^3 + 588z^2 - 337z + 108\sqrt{z} - 386 \right) \\
 & + 32\rho^5 \left( 18z^{7/2} + 144z^{5/2} + 216z^{3/2} + 108z^4 + 1105z^3 + 685z^2 - 1094z + 72\sqrt{z} - 344 \right) \\
 & - 8\rho^4 \left( 36z^{7/2} + 126z^{5/2} + 108z^{3/2} + 28z^5 + 810z^4 + 1760z^3 - 503z^2 - 1372z + 18\sqrt{z} - 147 \right) \\
 & + 2\rho^3 \left( 18z^{7/2} + 36z^{5/2} + 18z^{3/2} + 208z^5 + 1187z^4 + 469z^3 - 1519z^2 - 817z - 24 \right) \\
 & - 6144\rho^8 \left( 16z + 6\sqrt{z} - 9 \right) \quad (9.74)
 \end{aligned}$$

and

$$S_1 = \sqrt{1 - \frac{4\rho}{(1 - \sqrt{z})^2}}. \quad (9.75)$$

For the interference of process II and III we also have to introduce

$$S_2 = \sqrt{1 - \frac{4\rho}{(1 + \sqrt{z})^2}}. \quad (9.76)$$

In the limit  $\rho \rightarrow 0$  we obtain

$$\begin{aligned}
 \frac{d\sigma_{\text{square}}^{(2),\text{III}}}{ds'} = & \frac{\sigma^{(0)}(s')}{s} \left( \frac{\alpha}{4\pi} \right)^2 \left\{ \left[ \frac{4(1-z)(4+7z+4z^2)}{3z} + 8(1+z)\text{H}_0 \right] L^2 - \left[ \frac{128(1-z)(1+4z+z^2)}{9z} \right. \right. \\
 & \left. \left. + \frac{8(4+6z-3z^2-8z^3)}{3z}\text{H}_0 + 16(1+z)\text{H}_0^2 + \frac{16(1-z)(4+7z+4z^2)}{3z}\text{H}_1 + 32(1+z)\text{H}_{0,1} \right. \right. \\
 & \left. \left. - 32(1+z)\zeta_2 \right] L - \frac{2(1-z)}{27z(1+z)^2} (80 - 2463z - 5041z^2 - 2949z^3 - 163z^4) \right. \\
 & \left. - \left[ \frac{4}{9z(1+z)^3} (40 + 3z - 345z^2 - 445z^3 + 213z^4 + 318z^5 + 64z^6) \right. \right. \\
 & \left. \left. - \frac{64(1-z)(1+4z+z^2)}{3z}\text{H}_{-1} \right] \text{H}_0 - \frac{4(12+21z-27z^2-4z^3)}{3z}\text{H}_0^2 - 8(1+z)\text{H}_0^3 \right. \\
 & \left. + \left[ \frac{256(1-z)(1+4z+z^2)}{9z} + \frac{8(1-z)(4+7z+4z^2)}{3z}\text{H}_0 \right] \text{H}_1 + \frac{16(1-z)(4+7z+4z^2)}{3z}\text{H}_1^2 \right. \\
 & \left. + \left[ \frac{8(4+9z-3z^2-12z^3)}{3z} + 16(1+z)\text{H}_0 \right] \text{H}_{0,1} - \left[ \frac{64(1-z)(1+4z+z^2)}{3z} \right. \right.
 \end{aligned}$$

$$\begin{aligned}
 & - 64(1+z)H_0 \Big] H_{0,-1} + 32(1+z)H_{0,0,1} - 128(1+z)H_{0,0,-1} + 64(1+z)H_{0,1,1} \\
 & - \left[ \frac{8(8+3z+3z^2-16z^3)}{3z} + 48(1+z)H_0 \right] \zeta_2 \Big\} + \mathcal{O}\left(\frac{m^2}{s}L^2\right). \quad (9.77)
 \end{aligned}$$

The full process is therefore given by

$$\begin{aligned}
 \frac{d\sigma^{(2),\text{III}}}{ds'} &= \frac{\sigma^{(0)}(s')}{s} \left(\frac{\alpha}{4\pi}\right)^2 \left\{ \left[ \frac{4(1-z)(4+7z+4z^2)}{3z} + 8(1+z)H_0 \right] L^2 \right. \\
 &+ \left[ -\frac{128(1-z)(1+4z+z^2)}{9z} - \frac{8(4+6z-3z^2-8z^3)}{3z} H_0 - 16(1+z)H_0^2 \right. \\
 &- \left. \frac{16(1-z)(4+7z+4z^2)}{3z} H_1 - 32(1+z)H_{0,1} + 32(1+z)\zeta_2 \right] L \\
 &- \frac{2(1-z)}{27z(1+z)^2} (80 - 303z - 721z^2 - 789z^3 - 163z^4) \\
 &- \left( \frac{4}{9z(1+z)^3} (40 + 183z + 339z^2 + 527z^3 + 825z^4 + 462z^5 + 64z^6) \right. \\
 &- \left. \frac{16(4+27z+3z^2-4z^3)}{3z} H_{-1} + \frac{48(2+2z+z^2)}{z} H_{-1}^2 \right) H_0 \\
 &+ \left( \frac{4(-12-21z-12z^2+4z^3)}{3z} + \frac{40(2+2z+z^2)}{z} H_{-1} \right) H_0^2 - \frac{8}{3}(3+5z)H_0^3 \\
 &+ \left( \frac{256(1-z)(1+4z+z^2)}{9z} - \frac{8(-4-18z+15z^2+4z^3)}{3z} H_0 - \frac{8(4-6z+3z^2)}{z} H_0^2 \right) H_1 \\
 &+ \left( \frac{16(1-z)(4+7z+4z^2)}{3z} - \frac{4(4-6z+3z^2)}{z} H_0 \right) H_1^2 \\
 &+ \left( \frac{8(4-6z+9z^2-12z^3)}{3z} + \frac{8(8+7z^2)}{z} H_0 + \frac{8(4-6z+3z^2)}{z} H_1 \right) H_{0,1} \\
 &+ \left( \frac{16(-4-27z-3z^2+4z^3)}{3z} - \frac{32(5-2z)}{z} H_0 + \frac{96(2+2z+z^2)}{z} H_{-1} \right) H_{0,-1} \\
 &- \frac{32(2+z)}{z} H_{0,0,1} + \frac{16(10-18z-5z^2)}{z} H_{0,0,-1} - \frac{8(4-14z-5z^2)}{z} H_{0,1,1} \\
 &- \frac{96(2+2z+z^2)}{z} H_{0,-1,-1} + \left( \frac{8(-8+27z+16z^3)}{3z} + 16(7-3z)H_0 \right. \\
 &- \left. \frac{8(4-6z+3z^2)}{z} H_1 - \frac{48(2+2z+z^2)}{z} H_{-1} \right) \zeta_2 + 32(5+z)\zeta_3 \Big\} + \mathcal{O}\left(\frac{m^2}{s}L^2\right). \quad (9.78)
 \end{aligned}$$

This term does not only differ from Ref. [213] because of the squared term in Eq. (9.77) but also because of the wrong sign of the interference term, cf. Eq. (9.60), used in the original calculation. The difference is given by

$$\begin{aligned}
 \delta^{\text{III}} &= \frac{160}{3} - \frac{32}{z} + \frac{128}{3(1+z)^2} - \frac{64}{1+z} + 96(1+z)\zeta_3 - \left[ 52(1-z) + \frac{64}{3z}(1-z^3) \right] \ln^2(z) \\
 &- \frac{56}{3}(1+z)\ln^3(z) + \left[ 24(1-z) + 16(1+z)\ln(z) \right] \zeta_2 + \ln(z) \left[ \frac{104}{3} - \frac{32}{z} + \frac{128}{3(1+z)^3} \right]
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{256}{3(1+z)^2} - \frac{64}{1+z} + 64 \left( 1 - z + \frac{1-z^3}{3z} \right) \ln(1+z) \Big] - \left[ 40(1-z) + \frac{64}{3z}(1-z^3) \right. \\
 & \left. + 48(1+z) \ln(z) \right] \text{Li}_2(1-z) + 64 \left[ 1 - z + \frac{1}{3z}(1-z^3) - (1+z) \ln(z) \right] \text{Li}_2(-z) \\
 & + 128(1+z) \text{Li}_3(-z) - 96(1+z) S_{1,2}(1-z) + 2\delta_{\text{interf.}}^{\text{PS}}.
 \end{aligned} \tag{9.79}$$

The new result given in Eq. (9.78) is in full agreement with the result obtained in Ref. [214].

#### Process IV

The last contribution regarding the fermion pair production described in Ref. [213] is the interference between the diagrams of process II and process III. The integration can be performed in the same way as for the other processes. However, because of the more difficult topologies of the diagrams the contributing square roots are more involved and the iterated integrals need more letters. We therefore have to extend the alphabet used in this section by the following letters

$$d_{14} = \frac{1}{t(1-z) - 4\rho}, \tag{9.80}$$

$$d_{15} = \frac{1}{\sqrt{1-t(t(1-z) - 4\rho)}}, \tag{9.81}$$

$$d_{16} = \frac{1}{\sqrt{t(1-t)}\sqrt{t(1-z)^2 - 16\rho^2}}, \tag{9.82}$$

$$d_{17} = \frac{1}{\sqrt{t(1-t)}(t(1-z) - 4\rho)\sqrt{t(1-z)^2 - 16\rho^2}}, \tag{9.83}$$

$$d_{18} = \frac{1}{\sqrt{t}\sqrt{t(1-z)^2 - 16\rho^2}}, \tag{9.84}$$

$$d_{19} = \frac{1}{\sqrt{t}(t(1-z) - 4\rho)\sqrt{t(1-z)^2 - 16\rho^2}}, \tag{9.85}$$

$$d_{20} = \frac{1}{\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \tag{9.86}$$

$$d_{21} = \frac{1}{\sqrt{1-t}\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \tag{9.87}$$

$$d_{22} = \frac{\sqrt{t}}{\sqrt{t(1-z)^2 - 16\rho^2}\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \tag{9.88}$$

$$d_{23} = \frac{\sqrt{t}}{\sqrt{t(1-z)^2 - 16\rho^2}(t^2(1-z)^2 - 8\rho(1+z)t + 4tz + 16\rho^2)}, \tag{9.89}$$

$$d_{24} = \frac{1}{(t^2(1-z)^2 - 8\rho(1+z)t + 4tz + 16\rho^2)\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \tag{9.90}$$

$$d_{25} = \frac{t}{(t^2(1-z)^2 - 8\rho(1+z)t + 4tz + 16\rho^2)\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \tag{9.91}$$

$$d_{26} = \frac{1}{\sqrt{1-t}(t^2(1-z)^2 - 8\rho(1+z)t + 4tz + 16\rho^2)\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \tag{9.92}$$

$$d_{27} = \frac{t}{\sqrt{1-t}(t^2(1-z)^2 - 8\rho(1+z)t + 4tz + 16\rho^2)\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \tag{9.93}$$

$$d_{28} = \frac{1}{\sqrt{t}\sqrt{t(-1+z)^2 - 16\rho^2}\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \tag{9.94}$$

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$$d_{29} = \frac{1}{\sqrt{t}\sqrt{t(1-z)^2 - 16\rho^2}(t^2(1-z)^2 - 8\rho(1+z)t + 4tz + 16\rho^2)}, \quad (9.95)$$

$$d_{30} = \frac{1}{\sqrt{t}\sqrt{t(1-z)^2 - 16\rho^2}(t^2(1-z)^2 - 8\rho(1+z)t + 4tz + 16\rho^2)\sqrt{t^2(1-z)^2 - 8\rho(1+z)t + 16\rho^2}}, \quad (9.96)$$

$$d_{31} = \frac{\sqrt{t}}{\sqrt{t(1-z)^2 - 16\rho^2}(t^2(1-z)^2 - 8\rho(1+z)t + 4tz + 16\rho^2)\sqrt{t^2(1-z)^2 - 8\rho(1+z)t + 16\rho^2}}, \quad (9.97)$$

$$d_{32} = \frac{1}{t\sqrt{1-t}\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}, \quad (9.98)$$

$$d_{33} = \frac{t}{\sqrt{1-t}\sqrt{t^2(1-z)^2 - 8\rho t(1+z) + 16\rho^2}}. \quad (9.99)$$

For the full mass dependence we obtain

$$\begin{aligned} \frac{d\sigma^{(2),IV}}{ds'} &= \frac{\sigma^{(0)}(s')}{s} \left(\frac{\alpha}{4\pi}\right)^2 \left\{ -128z\tilde{H}_{v_4,d_{24}}P_{211} - 128(1-z)z\tilde{H}_{d_{13},d_{26}}P_{212} - 32(1-z)\tilde{H}_{d_{13},d_{32}}P_{212} \right. \\ &\quad - \frac{8(1-z^2)\tilde{H}_{d_{13},d_{21}}P_{213}}{\rho} - 256z\rho\tilde{H}_{d_{10},d_{24}}P_{217} + 512z\rho\tilde{H}_{d_9,d_{24}}P_{221} + \frac{512z\rho\tilde{H}_{d_{10},d_{26}}P_{222}}{S_2(1-\sqrt{z})^2} \\ &\quad + \frac{128\rho\tilde{H}_{d_{10},d_{32}}P_{222}}{S_2(1-\sqrt{z})^2} + \frac{512z\rho\tilde{H}_{d_{26},d_{10}}P_{222}}{S_2(1-\sqrt{z})^2} + \frac{128\rho\tilde{H}_{d_{32},d_{10}}P_{222}}{S_2(1-\sqrt{z})^2} + 32\tilde{H}_{0,d_{10}}P_{223} \\ &\quad - \frac{256z\tilde{H}_{d_{12},d_{26}}P_{228}}{1-z} - \frac{64\tilde{H}_{d_{12},d_{32}}P_{228}}{1-z} - \frac{16(1+z)\tilde{H}_{d_{12},d_{21}}P_{229}}{(1-z)\rho} + \frac{256z\tilde{H}_{d_{15},d_{24}}P_{231}}{1-z} \\ &\quad - \frac{64z\tilde{H}_{d_{15},d_{25}}P_{232}}{\rho} - \frac{32z\tilde{H}_{d_{25},d_{10}}P_{233}}{\rho} + 128z\tilde{H}_{d_{24},d_{10}}P_{225} \\ &\quad + \left[ 256z\frac{H_{v_3}}{\sqrt{1-4\rho}}P_{217} - 16(1-z)P_{217}\frac{H_{v_2}}{\sqrt{1-4\rho}} \right] \tilde{H}_{d_{10}} \\ &\quad + \left[ -\frac{16H_{v_2}P_{232}}{\rho\sqrt{1-4\rho}} - \frac{256zH_{v_3}P_{232}}{(-1+z)\rho\sqrt{1-4\rho}} \right] \tilde{H}_{d_{15}} + \left[ -\frac{8(1-z-4\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2\rho\sqrt{1-4\rho}} H_{v_2} \right. \\ &\quad + \left. \frac{128z(1-z-4\rho)P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2\rho\sqrt{1-4\rho}} H_{v_3} \right] \tilde{H}_{d_{16}} + \left[ -\frac{64(1-z-4\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2\sqrt{1-4\rho}} H_{v_2} \right. \\ &\quad + \left. \frac{1024z(1-z-4\rho)P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2\sqrt{1-4\rho}} H_{v_3} \right] \tilde{H}_{d_{17}} + \frac{8P_{227}}{3S_1^2(1-z)^2(1+\sqrt{z})^2} \tilde{H}_{d_{21}} \\ &\quad + \frac{128S_2z\rho P_{215}}{3S_1^2(1+\sqrt{z})^2} \tilde{H}_{d_{24}} - \frac{32S_2(1-\sqrt{z})zP_{210}}{3S_1^2(1+\sqrt{z})} \tilde{H}_{d_{25}} + \frac{128zP_{234}}{3S_1^2(1-z)^2(1+\sqrt{z})^2} \tilde{H}_{d_{26}} \\ &\quad - \frac{32zP_{230}}{3S_1^2(1-z)^2(1+\sqrt{z})^2} \tilde{H}_{d_{27}} + \left[ -\frac{128zH_{v_3}P_{214}}{\rho\sqrt{1-4\rho}} + \frac{8(1-z)H_{v_2}P_{214}}{\rho\sqrt{1-4\rho}} \right] \tilde{H}_{v_4} \\ &\quad + \frac{32P_{226}}{3S_1^2(1-z)(1+\sqrt{z})} \tilde{H}_{d_{32}} + \left[ \frac{32(1-z)H_{v_2}P_{221}}{\sqrt{1-4\rho}} - \frac{512zH_{v_3}P_{221}}{\sqrt{1-4\rho}} \right] \tilde{H}_{d_9} \\ &\quad - 4(7-3z+4z^2+16\rho)\tilde{H}_{d_{33}} + \left[ -\frac{32P_{214}\tilde{H}_{v_4}}{\rho\sqrt{1-4\rho}} + \frac{64\tilde{H}_{d_{10}}P_{217}}{\sqrt{1-4\rho}} - \frac{128\tilde{H}_{d_9}P_{221}}{\sqrt{1-4\rho}} \right. \end{aligned}$$



$$\begin{aligned}
 & + \frac{64P_{232}\tilde{H}_{d_{15}}}{(1-z)\rho\sqrt{1-4\rho}} - \frac{32S_2P_{215}}{3S_1^2(1+\sqrt{z})^2\sqrt{1-4\rho}} + \frac{32(1-z-4\rho)P_{235}\tilde{H}_{d_{16}}}{S_1^3(1-z)^2(1+\sqrt{z})^2\rho\sqrt{1-4\rho}} \\
 & + \frac{256(1-z-4\rho)P_{235}\tilde{H}_{d_{17}}}{S_1^3(1-z)^2(1+\sqrt{z})^2\sqrt{1-4\rho}} + 64(1-z)(1+z-10\rho+24\rho^2)\frac{\tilde{H}_{0,d_{10}}}{\sqrt{1-4\rho}} \\
 & + 128(1+z)^2\rho\frac{\tilde{H}_{0,d_{21}}}{\sqrt{1-4\rho}} - 2048z(1+z)\rho^2\frac{\tilde{H}_{0,d_{26}}}{\sqrt{1-4\rho}} - 512z(1+z)\rho(1+z-8\rho)\frac{\tilde{H}_{0,d_{27}}}{\sqrt{1-4\rho}} \\
 & - \frac{32(1+z+4\rho)\tilde{H}_{0,v_4}}{\sqrt{1-4\rho}} - \frac{512(1+z)\rho^2\tilde{H}_{0,d_{32}}}{\sqrt{1-4\rho}} + \frac{128(z-2\rho)(1+z-10\rho+24\rho^2)\tilde{H}_{0,d_9}}{\sqrt{1-4\rho}} \\
 & - \frac{256(1-z)(1-2\rho)^2(1+2\rho)\tilde{H}_{d_{14},d_{10}}}{\sqrt{1-4\rho}} + \frac{512(1-2\rho)^2(1+2\rho)(-z+2\rho)\tilde{H}_{d_{14},d_9}}{\sqrt{1-4\rho}} \\
 & + \frac{128(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{H}_{d_{18},d_{16}}}{\sqrt{1-4\rho}} + \frac{32(1+z)(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{21}}}{\sqrt{1-4\rho}} \\
 & + \frac{1024\rho(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{H}_{d_{18},d_{17}}}{\sqrt{1-4\rho}} - \frac{512z\rho(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{26}}}{\sqrt{1-4\rho}} \\
 & + \frac{512\rho(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{H}_{d_{19},d_{16}}}{(1-z)\sqrt{1-4\rho}} - \frac{128z(1+z-8\rho)(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{27}}}{\sqrt{1-4\rho}} \\
 & + \left. \frac{4096\rho^2(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{H}_{d_{19},d_{17}}}{(1-z)\sqrt{1-4\rho}} - \frac{128\rho(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{32}}}{\sqrt{1-4\rho}} \right] H_{v_1} \\
 & + \left[ \frac{8S_2(1-\sqrt{z})P_{215}}{3S_1^2(1+\sqrt{z})\sqrt{1-4\rho}} - \frac{16(1-z)^2(1+z-10\rho+24\rho^2)\tilde{H}_{0,d_{10}}}{\sqrt{1-4\rho}} \right. \\
 & - \frac{32(1-z)(1+z)^2\rho\tilde{H}_{0,d_{21}}}{\sqrt{1-4\rho}} + \frac{512(1-z^2)z\rho^2\tilde{H}_{0,d_{26}}}{\sqrt{1-4\rho}} + \frac{128(1-z^2)z\rho(1+z-8\rho)\tilde{H}_{0,d_{27}}}{\sqrt{1-4\rho}} \\
 & + \frac{8(1-z)(1+z+4\rho)\tilde{H}_{0,v_4}}{\sqrt{1-4\rho}} + \frac{128(1-z^2)\rho^2\tilde{H}_{0,d_{32}}}{\sqrt{1-4\rho}} - \frac{8(1-z^2)(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{21}}}{\sqrt{1-4\rho}} \\
 & - \frac{32(1-z)(z-2\rho)(1+z-10\rho+24\rho^2)\tilde{H}_{0,d_9}}{\sqrt{1-4\rho}} + \frac{64(1-z)^2(1-2\rho)^2(1+2\rho)\tilde{H}_{d_{14},d_{10}}}{\sqrt{1-4\rho}} \\
 & + \frac{128(1-z)(1-2\rho)^2(1+2\rho)(z-2\rho)\tilde{H}_{d_{14},d_9}}{\sqrt{1-4\rho}} + \frac{128(1-z)z\rho(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{26}}}{\sqrt{1-4\rho}} \\
 & - \frac{32(1-z)(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{H}_{d_{18},d_{16}}}{\sqrt{1-4\rho}} + \frac{32(1-z)\rho(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{32}}}{\sqrt{1-4\rho}} \\
 & - \frac{256(1-z)\rho(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{H}_{d_{18},d_{17}}}{\sqrt{1-4\rho}} \\
 & - \frac{128\rho(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{H}_{d_{19},d_{16}}}{\sqrt{1-4\rho}} \\
 & - \frac{1024\rho^2(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{H}_{d_{19},d_{17}}}{\sqrt{1-4\rho}} \\
 & \left. + \frac{32(1-z)z(1+z-8\rho)(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{27}}}{\sqrt{1-4\rho}} \right] H_{v_2} \\
 & + \left[ -\frac{128S_2zP_{215}}{3S_1^2(1+\sqrt{z})^2\sqrt{1-4\rho}} + \frac{256(1-z)z(1+z-10\rho+24\rho^2)\tilde{H}_{0,d_{10}}}{\sqrt{1-4\rho}} \right.
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{512z(1+z)^2\rho\tilde{H}_{0,d_{21}}}{\sqrt{1-4\rho}} - \frac{8192z^2(1+z)\rho^2\tilde{H}_{0,d_{26}}}{\sqrt{1-4\rho}} - \frac{2048z^2(1+z)\rho(1+z-8\rho)\tilde{H}_{0,d_{27}}}{\sqrt{1-4\rho}} \\
 & - \frac{128z(1+z+4\rho)\tilde{H}_{0,v_4}}{\sqrt{1-4\rho}} - \frac{2048z(1+z)\rho^2\tilde{H}_{0,d_{32}}}{\sqrt{1-4\rho}} + \frac{512z(z-2\rho)(1+z-10\rho+24\rho^2)\tilde{H}_{0,d_9}}{\sqrt{1-4\rho}} \\
 & - \frac{1024(1-z)z(1-2\rho)^2(1+2\rho)\tilde{H}_{d_{14},d_{10}}}{\sqrt{1-4\rho}} - \frac{2048z(1-2\rho)^2(1+2\rho)(z-2\rho)\tilde{H}_{d_{14},d_9}}{\sqrt{1-4\rho}} \\
 & + \frac{512z(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{H}_{d_{18},d_{16}}}{\sqrt{1-4\rho}} + \frac{128z(1+z)(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{21}}}{\sqrt{1-4\rho}} \\
 & + \frac{4096z\rho(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{H}_{d_{18},d_{17}}}{\sqrt{1-4\rho}} - \frac{2048z^2\rho(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{26}}}{\sqrt{1-4\rho}} \\
 & + \frac{2048z\rho(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{H}_{d_{19},d_{16}}}{(1-z)\sqrt{1-4\rho}} - \frac{512z\rho(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{32}}}{\sqrt{1-4\rho}} \\
 & + \frac{16384z\rho^2(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{H}_{d_{19},d_{17}}}{(1-z)\sqrt{1-4\rho}} \\
 & - \left. \frac{512z^2(1+z-8\rho)(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{27}}}{\sqrt{1-4\rho}} \right] H_{v_3} + \frac{32(1+z)(z-\rho+\rho^2)}{\rho}\tilde{H}_{0,d_{21}} \\
 & - 512z(z-\rho+\rho^2)\tilde{H}_{0,d_{26}} - \frac{128z(1+z-8\rho)(z-\rho+\rho^2)}{\rho}\tilde{H}_{0,d_{27}} - \frac{64(z-2\rho)P_{218}}{(1-z)}\tilde{H}_{0,d_9} \\
 & - 128(z-\rho+\rho^2)\tilde{H}_{0,d_{32}} + \frac{32(1+z)P_{219}}{S_2(1-\sqrt{z})^2}\tilde{H}_{d_{10},d_{21}} + 64(1-z)zP_{216}\tilde{H}_{d_{10},d_{25}} \\
 & - \frac{128z(1+z-8\rho)P_{219}}{S_2(1-\sqrt{z})^2}\tilde{H}_{d_{10},d_{27}} + \frac{64z(1+z-8\rho)P_{229}}{(1-z)\rho}\tilde{H}_{d_{12},d_{27}} \\
 & - \frac{128z(1-z-4\rho)P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2}\tilde{H}_{d_{16},d_{24}} - \frac{32z(1-z-4\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2\rho}\tilde{H}_{d_{16},d_{25}} + \frac{256z(z-2\rho)P_{225}}{(1-z)}\tilde{H}_{d_{24},d_9} \\
 & - \frac{1024z\rho(1-z-4\rho)P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2}\tilde{H}_{d_{17},d_{24}} - \frac{256z(1-z-4\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2}\tilde{H}_{d_{17},d_{25}} - \frac{8(1-z)P_{224}}{\rho}\tilde{H}_{d_{20},d_{10}} \\
 & + \frac{64(1+z)(z-2\rho)P_{219}}{S_2(1-\sqrt{z})^2(1-z)}\tilde{H}_{d_{21},d_9} - \frac{8(1-\sqrt{z})P_{235}}{S_1^3(1+\sqrt{z})\rho}\tilde{H}_{d_{22},d_{10}} + \frac{32(1+z)P_{219}}{S_2(1-\sqrt{z})^2}\tilde{H}_{d_{21},d_{10}} \\
 & - \frac{16(z-2\rho)P_{235}}{S_1^3(1+\sqrt{z})^2\rho}\tilde{H}_{d_{22},d_9} + \frac{16(1+z)(z-2\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2\rho} - \frac{16(z-2\rho)P_{224}}{\rho}\tilde{H}_{d_{20},d_9}\tilde{H}_{d_{23},d_{21}} \\
 & - \frac{256z(z-2\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2}\tilde{H}_{d_{23},d_{26}} - \frac{64z(z-2\rho)(1+z-8\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2\rho}\tilde{H}_{d_{23},d_{27}} \\
 & + \frac{1024z\rho(z-2\rho)P_{222}}{S_2(1-\sqrt{z})^2(1-z)}\tilde{H}_{d_{26},d_9} - \frac{64(z-2\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2}\tilde{H}_{d_{23},d_{32}} \\
 & - \frac{128z(1+z-8\rho)P_{219}}{S_2(1-\sqrt{z})^2}\tilde{H}_{d_{27},d_{10}} - \frac{256z(1+z-8\rho)(z-2\rho)P_{219}}{S_2(1-\sqrt{z})^2(1-z)}\tilde{H}_{d_{27},d_9} \\
 & + \frac{32(1-z)z(1+z-8\rho)P_{213}}{\rho}\tilde{H}_{d_{13},d_{27}} - \frac{64z(z-2\rho)P_{233}}{(1-z)\rho}\tilde{H}_{d_{25},d_9} \\
 & - \frac{32(z-\rho-z\rho)P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2\rho}\tilde{H}_{d_{28},d_{10}} + \frac{64(z-2\rho)(z-\rho-z\rho)P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2\rho}\tilde{H}_{d_{28},d_9}
 \end{aligned}$$

$$\begin{aligned}
& + \frac{128(1+z)\rho P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2} \tilde{H}_{d_{29},d_{21}} - \frac{2048z\rho^2 P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2} \tilde{H}_{d_{29},d_{26}} \\
& - \frac{512z\rho(1+z-8\rho)P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2} \tilde{H}_{d_{29},d_{27}} - \frac{512\rho^2 P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2} \tilde{H}_{d_{29},d_{32}} \\
& + \frac{512z\rho P_{235}}{S_1^3(1-z)(1+\sqrt{z})^2} \tilde{H}_{d_{30},d_{10}} + \frac{1024z\rho(z-2\rho)P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2} \tilde{H}_{d_{30},d_9} \\
& + \frac{128zP_{235}}{S_1^3(1-z)(1+\sqrt{z})^2} \rho (z-3\rho-3z\rho+8\rho^2) \tilde{H}_{d_{31},d_{10}} \\
& + \frac{256z(z-2\rho)P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2} \rho (z-3\rho-3z\rho+8\rho^2) \tilde{H}_{d_{31},d_9} \\
& + \frac{32(1-z)zP_{214}}{\rho} \tilde{H}_{v_4,d_{25}} + \frac{256\rho(z-2\rho)P_{222}}{S_2(1-\sqrt{z})^2(1-z)} \tilde{H}_{d_{32},d_9} \\
& + \frac{64(1+z)(z-2\rho)P_{219}}{S_2(1-\sqrt{z})^2(1-z)} \tilde{H}_{d_9,d_{21}} - 128(1-z)zP_{220} \tilde{H}_{d_9,d_{25}} + \frac{1024z\rho(z-2\rho)P_{222}}{S_2(1-\sqrt{z})^2(1-z)} \tilde{H}_{d_9,d_{26}} \\
& - \frac{256z(1+z-8\rho)(z-2\rho)P_{219}}{S_2(1-\sqrt{z})^2(1-z)} \tilde{H}_{d_9,d_{27}} + \frac{256\rho(z-2\rho)P_{222}}{S_2(1-\sqrt{z})^2(1-z)} \tilde{H}_{d_9,d_{32}} \\
& - 64(1-z)\rho(1+z+4\rho) \tilde{H}_{0,0,d_{10}} - 128\rho(z-2\rho)(1+z+4\rho) \tilde{H}_{0,0,d_9} \\
& - 256(1-z)z\rho(1+z-10\rho+24\rho^2) \tilde{H}_{0,d_{10},d_{24}} - 64(1-z)^2z(1+z-10\rho+24\rho^2) \tilde{H}_{0,d_{10},d_{25}} \\
& + 16(1-z)^2(1+z+4\rho) \tilde{H}_{0,d_{20},d_{10}} + 32(1-z)(z-2\rho)(1+z+4\rho) \tilde{H}_{0,d_{20},d_9} \\
& - 512z(1+z)^2\rho^2 \tilde{H}_{0,d_{21},d_{24}} - 128(1-z)z(1+z)^2\rho \tilde{H}_{0,d_{21},d_{25}} \\
& - 256(1-z)z\rho(1+z-10\rho+24\rho^2) \tilde{H}_{0,d_{24},d_{10}} - 512z(1+z)^2\rho^2 \tilde{H}_{0,d_{24},d_{21}} \\
& + 8192z^2(1+z)\rho^3 \tilde{H}_{0,d_{24},d_{26}} + 2048z^2(1+z)\rho^2(1+z-8\rho) \tilde{H}_{0,d_{24},d_{27}} \\
& + 2048z(1+z)\rho^3 \tilde{H}_{0,d_{24},d_{32}} - 512z\rho(z-2\rho)(1+z-10\rho+24\rho^2) \tilde{H}_{0,d_{24},d_9} \\
& - 64(1-z)^2z(1+z-10\rho+24\rho^2) \tilde{H}_{0,d_{25},d_{10}} - 128(1-z)z(1+z)^2\rho \tilde{H}_{0,d_{25},d_{21}} \\
& + 2048(1-z)z^2(1+z)\rho^2 \tilde{H}_{0,d_{25},d_{26}} + 512(1-z)z^2(1+z)\rho(1+z-8\rho) \tilde{H}_{0,d_{25},d_{27}} \\
& + 512(1-z)z(1+z)\rho^2 \tilde{H}_{0,d_{25},d_{32}} - 128(1-z)z(z-2\rho)(1+z-10\rho+24\rho^2) \tilde{H}_{0,d_{25},d_9} \\
& + 8192z^2(1+z)\rho^3 \tilde{H}_{0,d_{26},d_{24}} + 2048(1-z)z^2(1+z)\rho^2 \tilde{H}_{0,d_{26},d_{25}} \\
& + 2048z^2(1+z)\rho^2(1+z-8\rho) \tilde{H}_{0,d_{27},d_{24}} + 512(1-z)z^2(1+z)\rho(1+z-8\rho) \tilde{H}_{0,d_{27},d_{25}} \\
& + 128z\rho(1+z+4\rho) \tilde{H}_{0,v_4,d_{24}} + 32(1-z)z(1+z+4\rho) \tilde{H}_{0,v_4,d_{25}} \\
& + 2048z(1+z)\rho^3 \tilde{H}_{0,d_{32},d_{24}} + 512(1-z)z(1+z)\rho^2 \tilde{H}_{0,d_{32},d_{25}} \\
& - 512z\rho(z-2\rho)(1+z-10\rho+24\rho^2) \tilde{H}_{0,d_9,d_{24}} \\
& - 128(1-z)z(z-2\rho)(1+z-10\rho+24\rho^2) \tilde{H}_{0,d_9,d_{25}} \\
& + 1024(1-z)z\rho(1-2\rho)^2(1+2\rho) \tilde{H}_{d_{14},d_{10},d_{24}} + 256(1-z)^2z(1-2\rho)^2(1+2\rho) \\
& \times \tilde{H}_{d_{14},d_{10},d_{25}} + 1024(1-z)z\rho(1-2\rho)^2(1+2\rho) \tilde{H}_{d_{14},d_{24},d_{10}} + 2048z\rho(1-2\rho)^2(1+2\rho) \\
& \times (z-2\rho) \tilde{H}_{d_{14},d_{24},d_9} + 256(1-z)^2z(1-2\rho)^2(1+2\rho) \tilde{H}_{d_{14},d_{25},d_{10}} \\
& + 512(1-z)z(1-2\rho)^2(1+2\rho)(z-2\rho) \tilde{H}_{d_{14},d_{25},d_9} + 2048z\rho(1-2\rho)^2(1+2\rho)(z-2\rho) \\
& \times \tilde{H}_{d_{14},d_9,d_{24}} + 512(1-z)z(1-2\rho)^2(1+2\rho)(z-2\rho) \tilde{H}_{d_{14},d_9,d_{25}} + 32(1+z)(1-2\rho)(1+2\rho) \\
& \times (1-z-2\rho) \tilde{H}_{d_{15},d_{10},d_{21}} - 512z\rho(1-2\rho)(1+2\rho)(1-z-2\rho) \tilde{H}_{d_{15},d_{10},d_{26}}
\end{aligned}$$

9. Initial State Radiation to  $e^+ e^-$  Annihilation Revisited

$$\begin{aligned}
& -128z(1-2\rho)(1+2\rho)(1-z-2\rho)(1+z-8\rho)\tilde{\text{H}}_{d_{15},d_{10},d_{27}} \\
& -128\rho(1-2\rho)(1+2\rho)(1-z-2\rho)\tilde{\text{H}}_{d_{15},d_{10},d_{32}} \\
& +32(1+z)(1-2\rho)(1+2\rho)(1-z-2\rho)\tilde{\text{H}}_{d_{15},d_{21},d_{10}} \\
& -512z\rho(1-2\rho)(1+2\rho)(1-z-2\rho)\tilde{\text{H}}_{d_{15},d_{26},d_{10}} \\
& -128\rho(1-2\rho)(1+2\rho)(1-z-2\rho)\tilde{\text{H}}_{d_{15},d_{32},d_{10}} \\
& -128z(1-2\rho)(1+2\rho)(1-z-2\rho)(1+z-8\rho)\tilde{\text{H}}_{d_{15},d_{27},d_{10}} \\
& -\frac{1024z\rho(1-2\rho)(1+2\rho)(z-2\rho)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{15},d_{26},d_9} \\
& -\frac{256z(1-2\rho)(1+2\rho)(z-2\rho)(1-z-2\rho)(1+z-8\rho)}{1-z}\tilde{\text{H}}_{d_{15},d_{27},d_9} \\
& -\frac{256\rho(1-2\rho)(1+2\rho)(z-2\rho)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{15},d_{32},d_9} \\
& +\frac{64(1+z)(1-2\rho)(1+2\rho)(z-2\rho)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{15},d_9,d_{21}} \\
& -\frac{1024z\rho(1-2\rho)(1+2\rho)(z-2\rho)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{15},d_9,d_{26}} \\
& -\frac{64(1+z)(1-2\rho)(1+2\rho)(z-2\rho)(1-z-2\rho)}{-1+z}\tilde{\text{H}}_{d_{15},d_{21},d_9} \\
& -\frac{256z(1-2\rho)(1+2\rho)(z-2\rho)(1-z-2\rho)(1+z-8\rho)}{1-z}\tilde{\text{H}}_{d_{15},d_9,d_{27}} \\
& -\frac{256\rho(1-2\rho)(1+2\rho)(z-2\rho)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{15},d_9,d_{32}} \\
& -512z\rho(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{16},d_{24}} \\
& -128(1-z)z(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{16},d_{25}} \\
& -4096z\rho^2(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{17},d_{24}} \\
& -1024(1-z)z\rho(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{17},d_{25}} \\
& -32(1-z)^3(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{22},d_{10}} \\
& -64(1-z)^2(z-2\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{22},d_9} \\
& +64(1-z^2)(z-2\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{23},d_{21}} \\
& -1024(1-z)z\rho(z-2\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{23},d_{26}} \\
& -256(1-z)z(z-2\rho)(1+z-8\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{23},d_{27}} \\
& -256(1-z)\rho(z-2\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{23},d_{32}} \\
& -128(1-z)(z-\rho-z\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{28},d_{10}} \\
& -256(z-2\rho)(z-\rho-z\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{28},d_9} \\
& +512(1+z)\rho^2(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{29},d_{21}} \\
& -8192z\rho^3(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{29},d_{26}} \\
& -2048z\rho^2(1+z-8\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{29},d_{27}} \\
& -2048\rho^3(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{29},d_{32}} \\
& +2048(1-z)z\rho^2(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{30},d_{10}} \\
& +4096z\rho^2(z-2\rho)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{30},d_9} \\
& +512(1-z)z(z-3\rho-3z\rho+8\rho^2)(1+\rho-z\rho-3\rho^2)\tilde{\text{H}}_{d_{18},d_{31},d_{10}}
\end{aligned}$$

$$\begin{aligned}
 & + 1024z(z-2\rho)(1+\rho-z\rho-3\rho^2)(z-3\rho-3z\rho+8\rho^2)\tilde{\text{H}}_{d_{18},d_{31},d_9} \\
 & - \frac{2048z\rho^2(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)}{1-z}\tilde{\text{H}}_{d_{19},d_{16},d_{24}} \\
 & - 512z\rho(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{\text{H}}_{d_{19},d_{16},d_{25}} \\
 & - \frac{16384z\rho^3(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)}{1-z}\tilde{\text{H}}_{d_{19},d_{17},d_{24}} \\
 & - 4096z\rho^2(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{\text{H}}_{d_{19},d_{17},d_{25}} \\
 & - 128(1-z)^2\rho(1-4\rho^2)(1-z-2\rho)\tilde{\text{H}}_{d_{19},d_{22},d_{10}} \\
 & - 256(1-z)\rho(1-4\rho^2)(z-2\rho)(1-z-2\rho)\tilde{\text{H}}_{d_{19},d_{22},d_9} \\
 & + 256(1+z)\rho(1-4\rho^2)(z-2\rho)(1-z-2\rho)\tilde{\text{H}}_{d_{19},d_{23},d_{21}} \\
 & - 4096z\rho^2(1-4\rho^2)(z-2\rho)(1-z-2\rho)\tilde{\text{H}}_{d_{19},d_{23},d_{26}} \\
 & - 1024z\rho(1-4\rho^2)(z-2\rho)(1-z-2\rho)(1+z-8\rho)\tilde{\text{H}}_{d_{19},d_{23},d_{27}} \\
 & - 1024\rho^2(1-4\rho^2)(z-2\rho)(1-z-2\rho)\tilde{\text{H}}_{d_{19},d_{23},d_{32}} \\
 & - 512\rho(1-4\rho^2)(1-z-2\rho)(z-\rho-z\rho)\tilde{\text{H}}_{d_{19},d_{28},d_{10}} \\
 & - \frac{1024\rho(1-4\rho^2)(z-2\rho)(1-z-2\rho)(z-\rho-z\rho)}{1-z}\tilde{\text{H}}_{d_{19},d_{28},d_9} \\
 & + \frac{2048(1+z)\rho^3(1-4\rho^2)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{19},d_{29},d_{21}} \\
 & - \frac{32768z\rho^4(1-4\rho^2)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{19},d_{29},d_{26}} \\
 & - \frac{8192z\rho^3(1-4\rho^2)(1-z-2\rho)(1+z-8\rho)}{1-z}\tilde{\text{H}}_{d_{19},d_{29},d_{27}} \\
 & - \frac{8192\rho^4(1-4\rho^2)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{19},d_{29},d_{32}} \\
 & + 8192z\rho^3(1-4\rho^2)(1-z-2\rho)\tilde{\text{H}}_{d_{19},d_{30},d_{10}} \\
 & + \frac{16384z\rho^3(1-4\rho^2)(z-2\rho)(1-z-2\rho)}{1-z}\tilde{\text{H}}_{d_{19},d_{30},d_9} \\
 & + 2048z\rho(1-4\rho^2)(1-z-2\rho)(z-3\rho-3z\rho+8\rho^2)\tilde{\text{H}}_{d_{19},d_{31},d_{10}} \\
 & + \frac{4096z\rho(1-4\rho^2)(z-2\rho)(1-z-2\rho)}{1-z}(z-3\rho-3z\rho+8\rho^2)\tilde{\text{H}}_{d_{19},d_{31},d_9} \\
 & - 128z(1+z)\rho(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{21},d_{24}} - 32(1-z)z(1+z)(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{21},d_{25}} \\
 & - 128z(1+z)\rho(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{24},d_{21}} + 2048z^2\rho^2(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{24},d_{26}} \\
 & + 512z^2\rho(1+z-8\rho)(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{24},d_{27}} + 512z\rho^2(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{24},d_{32}} \\
 & - 32(1-z^2)z(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{25},d_{21}} + 512(1-z)z^2\rho(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{25},d_{26}} \\
 & + 128(1-z)z^2(1+z-8\rho)(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{25},d_{27}} \\
 & + 2048z^2\rho^2(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{26},d_{24}} + 512(1-z)z^2\rho(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{26},d_{25}} \\
 & + 512z^2\rho(1+z-8\rho)(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{27},d_{24}} \\
 & + 512z\rho^2(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{32},d_{24}} + 128(1-z)z\rho(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{32},d_{25}} \\
 & + 128(1-z)z\rho(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{25},d_{32}} \\
 & + 128(1-z)z^2(1+z-8\rho)(3+z^2-8\rho^2)\tilde{\text{H}}_{d_{20},d_{27},d_{25}} \\
 & - 16(1-z^2)(1+z-4\rho)\tilde{\text{H}}_{v_4,d_{10},d_{21}} + 256(1-z)z\rho(1+z-4\rho)\tilde{\text{H}}_{v_4,d_{10},d_{26}}
 \end{aligned}$$

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$$\begin{aligned}
& + 64(1-z)z(1+z-8\rho)(1+z-4\rho)\tilde{H}_{v_4,d_{10},d_{27}} \\
& + 64(1-z)\rho(1+z-4\rho)\tilde{H}_{v_4,d_{10},d_{32}} - 16(1-z^2)(1+z-4\rho)\tilde{H}_{v_4,d_{21},d_{10}} \\
& - 32(1+z)(z-2\rho)(1+z-4\rho)\tilde{H}_{v_4,d_{21},d_9} + 256(1-z)z\rho(1+z-4\rho)\tilde{H}_{v_4,d_{26},d_{10}} \\
& + 512z\rho(z-2\rho)(1+z-4\rho)\tilde{H}_{v_4,d_{26},d_9} + 64(1-z)z(1+z-8\rho)(1+z-4\rho)\tilde{H}_{v_4,d_{27},d_{10}} \\
& + 128z(z-2\rho)(1+z-4\rho)(1+z-8\rho)\tilde{H}_{v_4,d_{27},d_9} \\
& + 64(1-z)\rho(1+z-4\rho)\tilde{H}_{v_4,d_{32},d_{10}} + 128\rho(z-2\rho)(1+z-4\rho)\tilde{H}_{v_4,d_{32},d_9} \\
& - 32(1+z)(z-2\rho)(1+z-4\rho)\tilde{H}_{v_4,d_9,d_{21}} + 512z\rho(z-2\rho)(1+z-4\rho)\tilde{H}_{v_4,d_9,d_{26}} \\
& + 128z(z-2\rho)(1+z-4\rho)(1+z-8\rho)\tilde{H}_{v_4,d_9,d_{27}} \\
& + 128\rho(z-2\rho)(1+z-4\rho)\tilde{H}_{v_4,d_9,d_{32}} + \left[ -\frac{16P_{214}\tilde{H}_{v_4}}{\rho\sqrt{1-4\rho}} + \frac{32\tilde{H}_{d_{10}}P_{217}}{\sqrt{1-4\rho}} - \frac{64\tilde{H}_{d_9}P_{221}}{\sqrt{1-4\rho}} \right. \\
& + \frac{32\tilde{H}_{d_{15}}P_{232}}{(1-z)\rho\sqrt{1-4\rho}} - \frac{16S_2P_{215}}{3S_1^2(1+\sqrt{z})^2\sqrt{1-4\rho}} + \frac{16(1-z-4\rho)\tilde{H}_{d_{16}}P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2\rho\sqrt{1-4\rho}} \\
& + \frac{128(1-z-4\rho)\tilde{H}_{d_{17}}P_{235}}{S_1^3(1-z)^2(1+\sqrt{z})^2\sqrt{1-4\rho}} + \frac{32(1-z)(1+z-10\rho+24\rho^2)\tilde{H}_{0,d_{10}}}{\sqrt{1-4\rho}} \\
& - \frac{1024z(1+z)\rho^2\tilde{H}_{0,d_{26}}}{\sqrt{1-4\rho}} + \frac{256z(1+z)\rho(1+z-8\rho)\tilde{H}_{0,d_{27}}}{\sqrt{1-4\rho}} \\
& - \frac{16(1+z+4\rho)\tilde{H}_{0,v_4}}{\sqrt{1-4\rho}} - \frac{256(1+z)\rho^2\tilde{H}_{0,d_{32}}(z)}{\sqrt{1-4\rho}} - \frac{64z(1+z-8\rho)(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{27}}}{\sqrt{1-4\rho}} \\
& + \frac{64(z-2\rho)(1+z-10\rho+24\rho^2)\tilde{H}_{0,d_9}}{\sqrt{1-4\rho}} - \frac{128(1-z)(1-2\rho)^2(1+2\rho)\tilde{H}_{d_{14},d_{10}}}{\sqrt{1-4\rho}} \\
& - \frac{256(1-2\rho)^2(1+2\rho)(z-2\rho)\tilde{H}_{d_{14},d_9}}{\sqrt{1-4\rho}} + \frac{64(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{H}_{d_{18},d_{16}}}{\sqrt{1-4\rho}} \\
& + \frac{512\rho(1-z-4\rho)(1+\rho-z\rho-3\rho^2)\tilde{H}_{d_{18},d_{17}}}{\sqrt{1-4\rho}} + \frac{16(1+z)(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{21}}}{\sqrt{1-4\rho}} \\
& + \frac{256\rho(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{H}_{d_{19},d_{16}}}{(1-z)\sqrt{1-4\rho}} - \frac{256z\rho(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{26}}}{\sqrt{1-4\rho}} \\
& + \frac{2048\rho^2(1-4\rho^2)(1-z-2\rho)(1-z-4\rho)\tilde{H}_{d_{19},d_{17}}}{(1-z)\sqrt{1-4\rho}} + \frac{64(1+z)^2\rho\tilde{H}_{0,d_{21}}}{\sqrt{1-4\rho}} \\
& \left. - \frac{64\rho(3+z^2-8\rho^2)\tilde{H}_{d_{20},d_{32}}}{\sqrt{1-4\rho}} \right] \ln\left(\frac{1-z}{1+z}\right), \tag{9.101}
\end{aligned}$$

with the polynomials

$$P_{210} = -32\rho^2 - 44\rho + 6z^{3/2} + 19z^2 - 68\rho z + 144\rho\sqrt{z} - 20z - 6\sqrt{z} + 13, \tag{9.102}$$

$$P_{211} = -18\rho^2 + 9\rho + z^2 + 2\rho\sqrt{z}, \tag{9.103}$$

$$P_{212} = -6\rho^2 + 3\rho + 4z^2 - 2\rho z - 4z, \tag{9.104}$$

$$P_{213} = 6\rho^2 - 3\rho - 4z^2 + 2\rho z + 4z, \tag{9.105}$$

$$P_{214} = 18\rho^2 - 9\rho - z^2 - 2\rho\sqrt{z}, \tag{9.106}$$

$$P_{215} = 32\rho^2 + 44\rho - 6z^{3/2} - 19z^2 + 68\rho z - 144\rho\sqrt{z} + 20z + 6\sqrt{z} - 13, \tag{9.107}$$

$$P_{216} = -8\rho^2 + 2\rho - 2z^{3/2} + z^3 - 2\rho z^2 + z^2 - 8\rho^2 z + 4\rho z - 2z + 2\sqrt{z}, \tag{9.108}$$

$$P_{217} = 8\rho^2 - 2\rho + 2z^{3/2} - z^3 + 2\rho z^2 - z^2 + 8\rho^2 z - 4\rho z + 2z - 2\sqrt{z}, \tag{9.109}$$

$$P_{218} = -16\rho^3 + 16\rho^2 + 7\rho + 4\rho z^{3/2} + z^3 - 3\rho z^2 - z^2 - 16\rho^2 z - 4\rho\sqrt{z}, \quad (9.110)$$

$$P_{219} = -16\rho^3 + 16\rho^2 - 2\rho - 8\rho z^{3/2} - 5z^{5/2} + 4z^{3/2} + 2z^3 + 4\rho z^2 + 2z^2 - 8\rho^2 z - 8\rho^2\sqrt{z} + 2\rho z + 8\rho\sqrt{z} - 5z + 3\sqrt{z} - 1, \quad (9.111)$$

$$P_{220} = -16\rho^3 + 4\rho^2 - 2z^{3/2} + 2\rho z^2 + z^2 - 4\rho^2 z - 2\rho z + 4\rho\sqrt{z}, \quad (9.112)$$

$$P_{221} = 16\rho^3 - 4\rho^2 + 2z^{3/2} - 2\rho z^2 - z^2 + 4\rho^2 z + 2\rho z - 4\rho\sqrt{z}, \quad (9.113)$$

$$P_{222} = 16\rho^3 - 16\rho^2 + 2\rho + 8\rho z^{3/2} + 5z^{5/2} - 4z^{3/2} - 2z^3 - 4\rho z^2 - 2z^2 + 8\rho^2 z + 8\rho^2\sqrt{z} - 2\rho z - 8\rho\sqrt{z} + 5z - 3\sqrt{z} + 1, \quad (9.114)$$

$$P_{223} = 16\rho^3 - 16\rho^2 - 7\rho - 4\rho z^{3/2} - z^3 + 3\rho z^2 + z^2 + 16\rho^2 z + 4\rho\sqrt{z}, \quad (9.115)$$

$$P_{224} = 16\rho^3 - 16\rho^2 - 7\rho - 4\rho z^{3/2} + z^3 + 5\rho z^2 - z^2 + 16\rho^2 z - 4\rho z + 4\rho\sqrt{z}, \quad (9.116)$$

$$P_{225} = 48\rho^3 - 30\rho^2 - \rho - 4\rho z^{3/2} + z^3 + 11\rho z^2 - z^2 + 46\rho^2 z - 14\rho z + 4\rho\sqrt{z}, \quad (9.117)$$

$$P_{226} = 80\rho^3 - 184\rho^2 + 41\rho - 24\rho^2 z^{3/2} + 6\rho z^{5/2} + 75\rho z^{3/2} - 36z^{5/2} + 36z^{3/2} - 12\rho z^2 - 36z^2 + 76\rho^2 z + 68\rho^2\sqrt{z} - 169\rho z + 55\rho\sqrt{z} + 36z, \quad (9.118)$$

$$P_{227} = 384\rho^3 - 56\rho^2 - 38\rho + 80\rho^2 z^{5/2} + 192\rho^2 z^{3/2} + 100\rho z^{7/2} - 176\rho z^{5/2} + 212\rho z^{3/2} - 6z^{9/2} - 88z^{7/2} + 246z^{5/2} - 56z^{3/2} + 6z^5 - 78z^4 - 96\rho^2 z^3 + 126\rho z^3 + 99z^3 + 296\rho^2 z^2 - 346\rho z^2 + 119z^2 - 384\rho^3 z - 528\rho^2 z - 272\rho^2\sqrt{z} + 258\rho z + 56\rho\sqrt{z} - 57z + 7, \quad (9.119)$$

$$P_{228} = 12\rho^3 - 6\rho^2 + z^4 - 15\rho z^3 + 7z^3 - 10\rho^2 z^2 + 4\rho z^2 - 8z^2 - 28\rho^3 z + 16\rho^2 z + 15\rho z, \quad (9.120)$$

$$P_{229} = -12\rho^3 + 6\rho^2 - z^4 + 15\rho z^3 - 7z^3 + 10\rho^2 z^2 - 4\rho z^2 + 8z^2 + 28\rho^3 z - 16\rho^2 z - 15\rho z, \quad (9.121)$$

$$P_{230} = 1216\rho^3 - 136\rho^2 - 118\rho - 640\rho^3 z^{3/2} - 432\rho^2 z^{5/2} + 960\rho^2 z^{3/2} + 28\rho z^{7/2} - 192\rho z^{5/2} - 132\rho z^{3/2} + 30z^{9/2} - 220z^{7/2} + 426z^{5/2} - 164z^{3/2} + 24z^5 - 180\rho z^4 - 126z^4 + 288\rho^2 z^3 + 666\rho z^3 + 123z^3 + 192\rho^3 z^2 + 56\rho^2 z^2 - 1366\rho z^2 + 155z^2 + 128\rho^3 z + 640\rho^3\sqrt{z} - 592\rho^2 z - 1296\rho^2\sqrt{z} + 614\rho z + 104\rho\sqrt{z} - 99z + 24\sqrt{z} + 19, \quad (9.122)$$

$$P_{231} = -32\rho^4 + 56\rho^3 - 36\rho^2 + 6\rho + z^4 + 3\rho z^3 - 2z^3 - 12\rho^2 z^2 + 5\rho z^2 + z^2 - 56\rho^3 z + 56\rho^2 z - 14\rho z, \quad (9.123)$$

$$P_{232} = 32\rho^4 - 56\rho^3 + 36\rho^2 - 6\rho - z^4 - 3\rho z^3 + 2z^3 + 12\rho^2 z^2 - 5\rho z^2 - z^2 + 56\rho^3 z - 56\rho^2 z + 14\rho z, \quad (9.124)$$

$$P_{233} = 256\rho^4 - 192\rho^3 + 30\rho^2 + \rho - 4\rho z^{5/2} + 8\rho z^{3/2} - z^4 + 5\rho z^3 + 2z^3 + 34\rho^2 z^2 - 27\rho z^2 - z^2 + 256\rho^3 z - 96\rho^2 z + 21\rho z - 4\rho\sqrt{z}, \quad (9.125)$$

$$P_{234} = 192\rho^4 + 344\rho^3 - 94\rho^2 - \rho - 176\rho^3 z^{3/2} - 220\rho^2 z^{5/2} + 396\rho^2 z^{3/2} + 66\rho z^{7/2} - 116\rho z^{5/2} + 38\rho z^{3/2} - 72z^{7/2} + 144z^{5/2} - 72z^{3/2} + 24\rho z^4 - 36z^4 - 180\rho^2 z^3 + 159\rho z^3 + 36z^3 + 288\rho^3 z^2 + 270\rho^2 z^2 - 387\rho z^2 + 36z^2 + 192\rho^4 z - 632\rho^3 z - 16\rho^3\sqrt{z} - 92\rho^2 z - 272\rho^2\sqrt{z} + 205\rho z + 12\rho\sqrt{z} - 36z, \quad (9.126)$$

$$P_{235} = 256\rho^5 - 288\rho^4 + 144\rho^3 - 34\rho^2 + 3\rho - 64\rho^3 z^{3/2} - 16\rho^2 z^{5/2} + 80\rho^2 z^{3/2} + 2\rho z^{7/2} + 14\rho z^{5/2} - 22\rho z^{3/2} + 2z^{9/2} - 4z^{7/2} + 2z^{5/2} + z^5 - 5\rho z^4 - z^4 + 10\rho^2 z^3 + 20\rho z^3 - z^3 - 80\rho^3 z^2 - 22\rho^2 z^2 - 10\rho z^2 + z^2 + 160\rho^4 z - 128\rho^4\sqrt{z} - 128\rho^3 z + 64\rho^3\sqrt{z} + 78\rho^2 z - 32\rho^2\sqrt{z} - 8\rho z + 6\rho\sqrt{z}. \quad (9.127)$$

In the limit  $\rho \ll 1$  this term reduces to

$$\begin{aligned}
 \frac{d\sigma^{(2),IV}}{ds'} &= \frac{\sigma^{(0)}(s')}{s} \left(\frac{\alpha}{4\pi}\right)^2 \left\{ - \left[ 8(8-7z) + \frac{8(5-2z^2)}{1-z} H_0 + \frac{8(1+z^2)}{1-z} (H_0^2 + 2H_0H_1 \right. \right. \\
 &\quad \left. \left. - 2H_{0,1} + 2\zeta_2) \right] L + \frac{8(27-42z+23z^2)}{1-z} + \left[ \frac{8}{(1-z)^2(1+z)} (3+10z-11z^2+22z^3-8z^4) \right. \right. \\
 &\quad \left. \left. + \frac{64(1+z)}{1-z} H_{-1} \right] H_0 - \frac{8(1+z)^2}{1-z} H_0^2 - \frac{8(1+2z^2)}{3(1-z)} H_0^3 + \left[ 16(8-7z) - \frac{8(3-2z-2z^2)}{1-z} H_0 \right. \right. \\
 &\quad \left. \left. + \frac{16(2+z^2)}{1-z} H_0^2 \right] H_1 + \frac{16}{1-z} H_0 H_1^2 + \left[ \frac{8(13-2z-6z^2)}{1-z} - \frac{16(5+4z^2)}{1-z} H_0 + \frac{32z^2}{1-z} H_1 \right] H_{0,1} \right. \\
 &\quad \left. - \left[ \frac{64(1+z)}{1-z} - \frac{32(1+z^2)}{1-z} H_0 \right] H_{0,-1} + \frac{128(1+z^2)}{1-z} H_{0,0,1} - \frac{64(1+z^2)}{1-z} H_{0,0,-1} \right. \\
 &\quad \left. - \frac{32(1+2z^2)}{1-z} H_{0,1,1} - \left[ \frac{24(3-2z-2z^2)}{1-z} + \frac{16(2+3z^2)}{1-z} H_0 + \frac{32z^2}{1-z} H_1 \right] \zeta_2 \right. \\
 &\quad \left. - \frac{16(3+z^2)}{1-z} \zeta_3 \right\} + \mathcal{O}\left(\frac{m^2}{s}L\right). \tag{9.128}
 \end{aligned}$$

The difference with regard to the result given in Ref. [213] is given by

$$\begin{aligned}
 \delta_{IV} &= \frac{2(53+994z+32z^2+742z^3-85z^4-8z^5)}{9(1-z)(1+z)^2} - 8 \left[ \frac{1-14z-56z^2+78z^3-25z^4}{(1-z^2)^2} \right. \\
 &\quad \left. + \frac{1+z^2}{1-z} \ln(z) \right] \zeta_2 - \frac{8z(13+12z^2-20z^3+3z^4)}{(1-z^2)^2} \ln^2(z) + 16 \left[ \frac{1-z+7z^2-3z^3}{(1+z)^2} \right. \\
 &\quad \left. + \frac{7+3z^2}{2(1-z)} \ln(z) \right] \text{Li}_2(1-z) + \left[ \frac{32(1+5z-4z^2)}{(1-z)^2} \ln(1+z) \right. \\
 &\quad \left. - \frac{16(4-7z-6z^2-128z^3+2z^4-9z^5)}{3(1-z)^2(1+z)^3} \right] \ln(z) + \frac{32(1+5z-4z^2)}{(1-z)^2} \text{Li}_2(-z). \tag{9.129}
 \end{aligned}$$

Since the interference contribution cannot be associated with an operator matrix element there is no direct comparison with Ref. [214]. It appears as one part of process I given there.

### Further Contributions

Besides the processes II-IV there are also other contributions to the fermion pair production not considered in Ref. [213] but contained in Ref. [421]. These contributions are given by the diagrams in Fig. 9.6 and their interference with the diagrams in Figs. 9.4 and 9.5. These contributions do

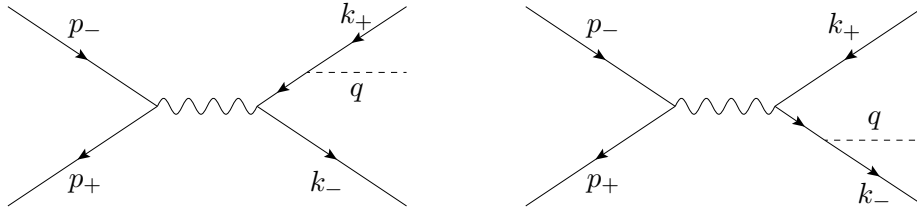


Figure 9.6.: Diagrams representing the contributions neglected in [213] but contained in [421].



not contain mass singularities and can therefore be computed like the interference contribution to process III by directly taking the limit  $\rho \rightarrow 0$ .

For the contributions from Fig. 9.6 we find

$$\begin{aligned} \frac{d\sigma^{(2),\text{BB}}}{ds'} &= \frac{\sigma^{(0)}(s')}{s} \left(\frac{\alpha}{4\pi}\right)^2 \left\{ \frac{40}{3}(1-z^2) + \left[ \frac{8}{3}(3+4z+3z^2) \right. \right. \\ &\quad \left. \left. - \frac{32}{3}(1+z)^2\text{H}_{-1} \right] \text{H}_0 + \frac{8}{3}(1+z)^2\text{H}_0^2 + \frac{32}{3}(1+z)^2\text{H}_{0,-1} - \frac{16}{3}(1+z)^2\zeta_2 \right\} + \mathcal{O}\left(\frac{m^2}{s}\right) \end{aligned} \quad (9.130)$$

and for the interference between the diagrams in Figs. 9.6 and 9.5 we obtain

$$\begin{aligned} \frac{d\sigma^{(2),\text{BC}}}{ds'} &= \frac{\sigma^{(0)}(s')}{s} \left(\frac{\alpha}{4\pi}\right)^2 \left\{ 2(1-z)(27+13z) + \left[ 4(9+11z) + 24(1+z)^2\text{H}_{-1} \right. \right. \\ &\quad \left. \left. - 24(1+z)^2\text{H}_{-1}^2 \right] \text{H}_0 + \left[ 2(6-8z-15z^2) + 20(1+z)^2\text{H}_{-1} \right] \text{H}_0^2 + \frac{4}{3}(1+4z+z^2)\text{H}_0^3 \right. \\ &\quad \left. + 36(1-z^2)\text{H}_0\text{H}_1 - \left[ 36(1-z^2) - 16(1+3z+z^2)\text{H}_0 \right] \text{H}_{0,1} - \left[ 24(1+z)^2 \right. \right. \\ &\quad \left. \left. + 24(1+z)^2\text{H}_0 - 48(1+z)^2\text{H}_{-1} \right] \text{H}_{0,-1} - 32(1+3z+z^2)\text{H}_{0,0,1} + 8(1+z)^2\text{H}_{0,0,-1} \right. \\ &\quad \left. - 48(1+z)^2\text{H}_{0,-1,-1} + \left[ 24(2-z)(1+z) + 8(3+8z+3z^2)\text{H}_0 - 24(1+z)^2\text{H}_{-1} \right] \zeta_2 \right. \\ &\quad \left. + 32(1+3z+z^2)\zeta_3 \right\} + \mathcal{O}\left(\frac{m^2}{s}\right) \end{aligned} \quad (9.131)$$

These results are in full agreement with Ref. [421], from which we also adopted the notation for the different contributions. The interference between the diagrams in Figs. 9.6 and 9.4 does only contribute for axial couplings and will not be considered here.

### Numerical Results

The relative deviations for the results for processes II-IV in the present calculation and Ref. [213] are shown in Figure 9.7. Here  $\Delta_{(2)}$  denotes the ratio of the difference terms  $\delta_i$  given in Eqs. (9.37,9.79,9.129) and the corresponding complete  $\mathcal{O}(\alpha^2)$  correction for  $i = \text{II}, \text{III}, \text{IV}$ . All illustrations are made for  $z < 1$ . The relative differences reach from +25 to -60% for  $z \in [10^{-5}, 1]$ . Here we have changed the term  $\ln(z)/(1-z)^2 \rightarrow \ln^2(z)/(1-z)^2$  in Eq. (2.43) of Ref. [213] which appears twice (suggesting a typo), such that this term is only logarithmic but not linear divergent for  $z \rightarrow 1$  and thus integrable. Otherwise the difference would be even larger.

Figure 9.8 shows the different contributions at  $\mathcal{O}(\alpha^2)$  of initial state  $e^+e^-$  pair production to  $\gamma^*/Z^*$ -boson production. The dominant contributions come from the pure singlet and non-singlet terms, other contributions are smaller but not negligible at the 0.1% level in the radiator function. For large values of  $z = \frac{s'}{s}$  the non-singlet terms are dominant, whereas for  $z \lesssim 0.03$  the pure singlet contributions dominate.

### 9.3.2. Corrections due to Photon Emission

Following Ref. [213], the  $\mathcal{O}(\alpha^2)$  correction due to photon emission can be split up into the following six parts:

- $\delta_2^{S2}$ , both photons are soft;
- $\delta_2^{V2}$ , both photons are virtual;
- $\delta_2^{S1V1}$ , one photon is soft, one virtual;
- $\delta_2^{S1H1}$ , one photon is soft, one hard;
- $\delta_2^{V1H1}$ , one photon is virtual, one hard;
- $\delta_2^{H2}$ , both photons are hard.

The complete cross section can be expressed as

$$\begin{aligned} \frac{d\sigma}{ds'} = \frac{\sigma^{(0)}}{s} \left(\frac{\alpha}{\pi}\right)^2 & \left\{ \delta(1-z) \left[ \delta_2^{S2}(\varepsilon, \lambda) + \delta_2^{V2}(\lambda) + \delta_2^{S1V1}(\varepsilon, \lambda) \right] \right. \\ & \left. + \theta(1-z-\varepsilon) \left[ \delta_2^{S1H1}(\varepsilon, \lambda, z) + \delta_2^{V1H1}(\lambda, z) + \delta_2^{H2}(\varepsilon, z) \right] \right\}. \end{aligned} \quad (9.132)$$

The virtual part, in the asymptotic limit, is again given by the form factor  $F_1$

$$\delta_2^{S2}(\varepsilon, \lambda) = |F_1^{(1)}|^2 + 2\text{Re}(F_1^{(2)}). \quad (9.133)$$

The explicit expressions can be found in Refs. [213, 427, 428].

If only one photon is soft, the cross section factorizes into the  $\mathcal{O}(\alpha)$  soft and hard (virtual) emission

$$\delta_2^{S1H1}(\varepsilon, \lambda, z) = \delta_1^{S1}(\varepsilon, \lambda) \delta_1^{H1}(z), \quad (9.134)$$

$$\delta_2^{S1V1}(\varepsilon, \lambda) = \delta_1^{S1}(\varepsilon, \lambda) \delta_1^{V1}(\lambda). \quad (9.135)$$

This can most easily be seen by explicitly factorizing the phase space in this limit, cf. Ref. [213].

If both photons are soft the factorization is not complete. Since the two photons are not uncorrelated one has to introduce a correction factor, which can also be understood on the level of phase space factorization. The double soft emission is then given by

$$\delta_2^{S2} = \frac{1}{2} \left( \delta_1^{S1} \right)^2 - 2(L-1)^2 \zeta_2. \quad (9.136)$$

The factor of  $\frac{1}{2}$  emerges, since the photons are indistinguishable. For the soft photon parts we completely agree with the results presented in Ref. [213]. The contributions due to one virtual and one hard photon  $\delta_2^{V1H1}$  and due to two hard photons  $\delta_2^{H2}$  are still work in progress. For the virtual-hard contributions a large amount of scalar one loop diagrams has already been computed, only the contribution from the box diagrams are still work in progress. For the hard radiation we had to employ a regularization at the phase space boundaries so we can expand in the mass ratio without interference of the soft-hard separator. The logarithmic corrections due to this separator have been already confirmed. After the last two corrections are finished the full corrections due to  $\mathcal{O}(\alpha^2)$  initial state radiations can be applied to several observables. The most prominent ones are the  $Z$ -production  $e^+ e^- \rightarrow Z$ , but also the determination of the  $t\bar{t}$  resonance and Higgs production cross sections will benefit from the precise knowledge of these corrections. Furthermore we can add the contributions due to axial-vector couplings without dealing with  $\gamma_5$  in  $d$  dimensions, since the calculation can be done in  $d = 4$  rigorously.

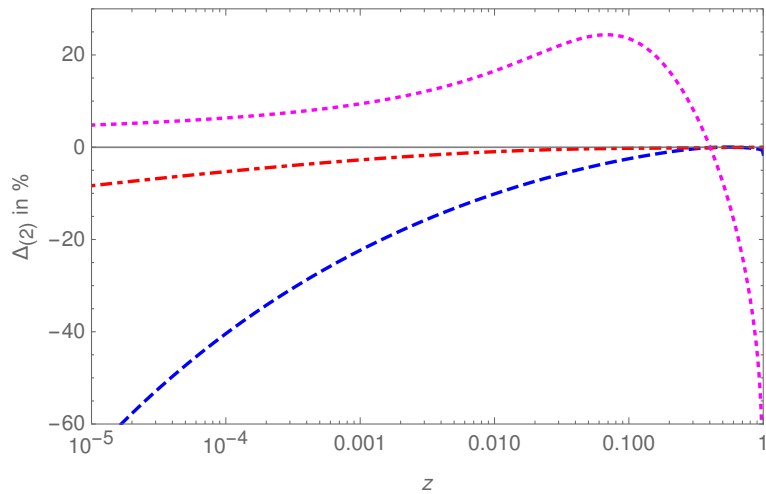


Figure 9.7.: Relative deviations of the results of Ref. [213] from the exact result in % for the  $\mathcal{O}(\alpha^2)$  corrections. The non-singlet contribution (process II): dash-dotted line; the pure singlet contribution (process III): dashed; the interference term between both contributions (process IV): dots; for  $s = M_Z^2$ ,  $M_Z = 91.1879$  GeV.

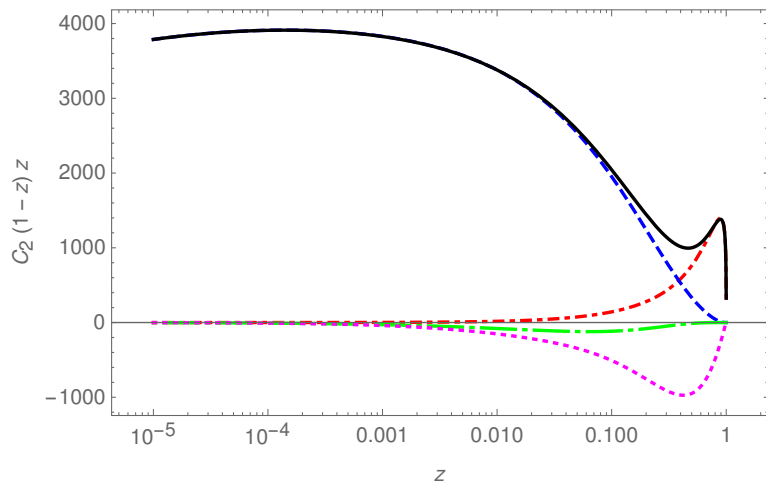


Figure 9.8.: The initial state  $\mathcal{O}(\alpha^2)$  corrections to  $\gamma^*/Z^*$  production due to  $e^+e^-$  pair production multiplied by  $z(1-z)$ . The non-singlet contribution (process II): dash-dotted line; the pure singlet contribution (process III): dashes; the interference term between both contributions (process IV)  $\times 10$ : dotted; the vector contributions implied by Eqs. (9.130,9.131)  $\times 100$ : long dash-dotted; all contributions: full line for  $s = M_Z^2$ .



## 10. Conclusion and Outlook

To fully exploit the precise data on the structure function  $F_2(x, Q^2)$  taken by HERA the knowledge of the NNLO heavy quark effects are important. They will enable us to extract important parameters of the Standard Model, foremost the heavy quark masses  $m_c$  and  $m_b$  and the strong coupling constant  $\alpha_s(M_Z)$  as well as the PDFs of the proton more precisely. In the asymptotic region,  $Q^2 \gg m^2$ , these effects can be described by universal massive operator matrix elements and massless Wilson coefficients, using factorization in this limit. In the single mass case all OMEs except of  $A_{Qg}$  have already been calculated analytically. Since the charm and the bottom mass do not form a strong hierarchy it is also necessary to include the effect of both heavy quarks simultaneously instead of decoupling them one after another. The massive OMEs can also be used to define the VFNS scheme which is an important ingredient to obtain precise and reliable PDFs for the LHC. This thesis aim is to deepen the understanding of mass effects through explicit calculations and to take further steps to the completion of the massive OMEs at NNLO.

In Chapter 3 we calculate the full mass dependence of the unpolarized pure singlet Wilson coefficients at NLO analytically, which has only been available in numeric form before. It is possible to express the result via iterated integrals of square root valued letters. We proof the asymptotic factorization into massless Wilson coefficient and massive operator matrix element by explicit expansion of the analytic result in the asymptotic limit. This also allows us to obtain the asymptotic series in the power corrections up to order  $(m^2/Q^2)^2$ , expanding the kinematic reach of the approximations. More coefficients in the asymptotic series can be computed easily if needed. Since the coefficients of the expansion are given by simple HPLs these results can be used for a fast evaluation of the Wilson coefficients up to lower values of the virtuality. This is especially useful for the longitudinal Wilson coefficient  $H_L^{(2),PS}$ , since the asymptotic representation in only values for quite high virtualities  $Q^2 \gtrsim 800m^2$ . Our power suppressed expansion coefficients can be applied for much lower virtualities  $Q^2 \gtrsim 20m^2$  for low value of  $x$ . In Chapter 4 we extend this treatment to the polarized pure singlet Wilson coefficient  $g_1^{(2),PS}$ . The techniques introduced in this chapters can in principle also be used to obtain the full mass dependence of the gluonic Wilson coefficient.

We turn to the renormalization of two-mass effects OMEs up to NNLO and correct some inconsistencies in the literature in Chapter 5. During the work on the renormalization we realized that the simultaneous decoupling of charm and bottom quarks also introduces two-mass effects at NLO through reducible contributions, although genuine diagrams with two heavy quarks only contribute from NNLO onwards. With these results, we extend the VFNS in Chapter 6 to include these two-mass effects. We also illustrate their numerical impact on the PDFs. The correct treatment of the VFNS is a crucial step to obtain precise and stable PDFs for the use at the LHC.

In Chapter 7 the two-mass effects to the unpolarized pure singlet and gluonic OMEs at NNLO are calculated analytically in momentum fraction and, in the latter case, also in Mellin space. The gluonic operator matrix element in Mellin space is composed of harmonic, generalized harmonic, cyclotomic and generalized binomially weighted sums. Their inversion to momentum fraction space introduces iterated integrals over square root valued letters which additionally depend on the mass ratio  $\eta$ . In the pure singlet case we also need iterated integrals over square root valued arguments to express the result in momentum fraction space, however, we also find a new class of functions with restricted support in the momentum fraction. Furthermore, we extend the algorithm to calculate arbitrary large moments to treat also two-scale problems in the expansion in one of the scales. Using this algorithm a thousand moments of the unpolarized two-mass contributions to the OME  $A_{Qg}$ , expanded up to

$\mathcal{O}(\eta^5)$ , have been completed. This brings the two-mass contributions to a similar status as the single mass contributions for which also a large number of moments have been computed. These moments can already be used for phenomenological analyses in Mellin space. In future work, they can also be used to obtain more information about the analytic structure of the in  $\eta$  expanded OME using guessing techniques. With the completion of these OMEs only the momentum space solution of the gluonic OME  $A_{gg,Q}^{(3)}$  and the analytic solution of  $A_{Qg}$  are missing. However, the analytic solution of  $A_{Qg}$  in the single- and two-mass contains objects which recurrences in Mellin space or differential equations in momentum fraction space do not factorize to first order and therefore require more general solution spaces than the ones defined in Appendix C. In momentum fraction space this leads to complete elliptic integrals and more general functions.

A new projector for the calculation of polarized OMEs with external light quarks is presented in Chapter 8. This projector allows to calculate the polarized OMEs consistently in the Larin scheme using the same techniques as has been used for the unpolarized case. Using this projector we calculate missing OMEs at NLO up to  $\mathcal{O}(\varepsilon)$ . Also first result at NNLO in the single and two-mass case are presented. These results are the first independent cross-check of the  $\mathcal{O}(T_F)$  part of the NNLO polarized anomalous dimensions calculated in Ref. [158]. The calculation of the full set of polarized anomalous dimensions at  $\mathcal{O}(T_F)$  is currently under way. Furthermore, with this new results the VFNS in the polarized case can be established.

In Chapter 9 we address the long standing discrepancy between two calculations of QED initial state radiation to  $e^+e^-$  annihilation into a neutral vector boson at  $\mathcal{O}(\alpha^2)$ , cf. Refs. [213, 214]. We integrate the phase space for fermion pair radiation exactly without any approximation and subsequently expand in  $m^2/s$ . We find agreement with the calculation based on asymptotic factorization. This result proofs the factorization of massive external particles in this process. Numerically these results show significant deviations from the ones obtained in Ref. [213], which have been implemented in many analyses of the  $Z$ -peak and other virtual gauge boson mediated processes. The corrections due to photon radiation are currently work in progress, here the double hard radiation and the virtual-hard contributions have to be recalculated. We agree with the soft photon contributions. When these calculations are finished, these results will provide important input for proposed  $e^+e^-$  colliders. Their planned high luminosities will require very precise theoretical input to match this experimental precision. This is not only the case for  $Z$ -boson production and the precise determination of electroweak parameters, but also for the  $t\bar{t}$  resonance or Higgs boson production.

The calculations presented in this thesis have greatly profited from a strong collaboration with mathematicians and experts in computer algebra. Although problems which factorize to first order in either Mellin or momentum fraction space can nowadays be handled in an automated way, this class of problems is not general enough to cover the involved calculations needed to keep up with the experimental precision delivered by the LHC experiments and what is promised by future collider generations. Here two important topics can be identified. On the one hand, factors which do not factorize to first order have to be dealt with in an automated fashion. In order to do so the corresponding function spaces have to be understood more deeply. On the other hand, multi-scale problems, even at relatively low loop order, are problematic to deal with using current technologies. Here our treatment of direct phase space integration in differential fields could be further refined to tackle the integration of even more involved phase spaces.

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Last but not least, I would like to thank my family and friends for their constant support, encouragement and faith throughout the years.





# A. Notation and Conventions

In this thesis natural units, i.e.

$$\hbar = 1, \quad c = 1, \quad \varepsilon_0 = 1 \quad (\text{A.1})$$

with Planck's constant  $\hbar$ , the speed of light  $c$  and the permittivity of the vacuum  $\varepsilon_0$ , are used.

For dimensional regularization the dimension of space-time is set to  $d = 4 + \varepsilon$  and we use the 'mostly minus' definition of the Minkowski metric

$$g_{\mu\nu} = \text{diag}(1, -1, \dots, -1). \quad (\text{A.2})$$

Furthermore, we use for the inner product in Minkowski space interchangeably

$$p \cdot q = p_\mu q^\mu = \sum_{\mu=0}^{d-1} p_\mu q^\mu. \quad (\text{A.3})$$

Accordingly, we use Einstein's summation convention unless stated otherwise.

The Dirac matrices  $\gamma_\mu$  are defined through their anti-commutation relations

$$\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}, \quad (\text{A.4})$$

where the Lorentz indices are  $d$ -dimensional.

The bi-spinors  $u$  and  $v$  are solutions to the free Dirac-equation

$$(\not{p} - m)u(p) = 0, \quad \bar{u}(p)(\not{p} - m) = 0 \quad (\text{A.5})$$

$$(\not{p} + m)v(p) = 0, \quad \bar{v}(p)(\not{p} + m) = 0 \quad (\text{A.6})$$

and are normalized to

$$\sum_{\sigma=\pm 1/2} u(p, \sigma)\bar{u}(p, \sigma) = \not{p} + m, \quad (\text{A.7})$$

$$\sum_{\sigma=\pm 1/2} v(p, \sigma)\bar{v}(p, \sigma) = \not{p} - m. \quad (\text{A.8})$$

For the polarization vectors of external gluons we use

$$\sum_{\sigma=-1,0,1} \epsilon_\mu(p, \sigma)\epsilon_\nu^*(p, \sigma) = -g_{\mu\nu}, \quad (\text{A.9})$$

where  $\sigma$  represents the spin of the respective particle.

The non-Abelian gauge group of QCD introduces the generators  $t_i$  of the associated Lie algebra into the Feynman rules. In the following we comprise our conventions for the colour algebra of a general  $SU(N)$  gauge group. The Lie algebra is defined by the commutation relations of its generators

$$[t^a, t^b] = if^{abc}t^c \quad (\text{A.10})$$

### A. Notation and Conventions

where  $f^{abc}$  are the structure constants and totally anti-symmetric in all indices. The anti-commutation relations can be defined with the totally symmetric structure constants  $d^{abc}$  via

$$\{t^a, t^b\} = \frac{\delta^{ab}}{N} + d^{abc}t^c. \quad (\text{A.11})$$

Most color structures can be expressed by the following invariants

$$f^{abc}f^{abd} = C_A\delta^{cd}, \quad (\text{A.12})$$

$$t_{ij}^a t_{jl}^a = C_F\delta_{il}, \quad (\text{A.13})$$

$$t_{ij}^a t_{ji}^b = T_F\delta^{ab} \quad (\text{A.14})$$

which for QCD's  $SU(3)$  take the values  $C_A = 3$ ,  $C_F = 4/3$  and  $T_F = 1/2$ .

## B. Feynman Rules

We use the QCD Feynman rules of Ref. [70], which for completeness can be found in Figure B.1. We label  $d$ -dimensional momenta by  $p_i$  and an arrow in the direction of momentum transfer. Lorentz-indices are denoted by Greek letters  $\mu, \nu, \dots$  and color indices in the adjoint representation are  $a, b, \dots$  while the ones in the fundamental one are denoted by  $i, j$ . Solid lines represent fermions, wavy lines gluons and dashed lines ghosts. A factor of  $(-1)$  has to be included for each closed fermion or ghost loop.

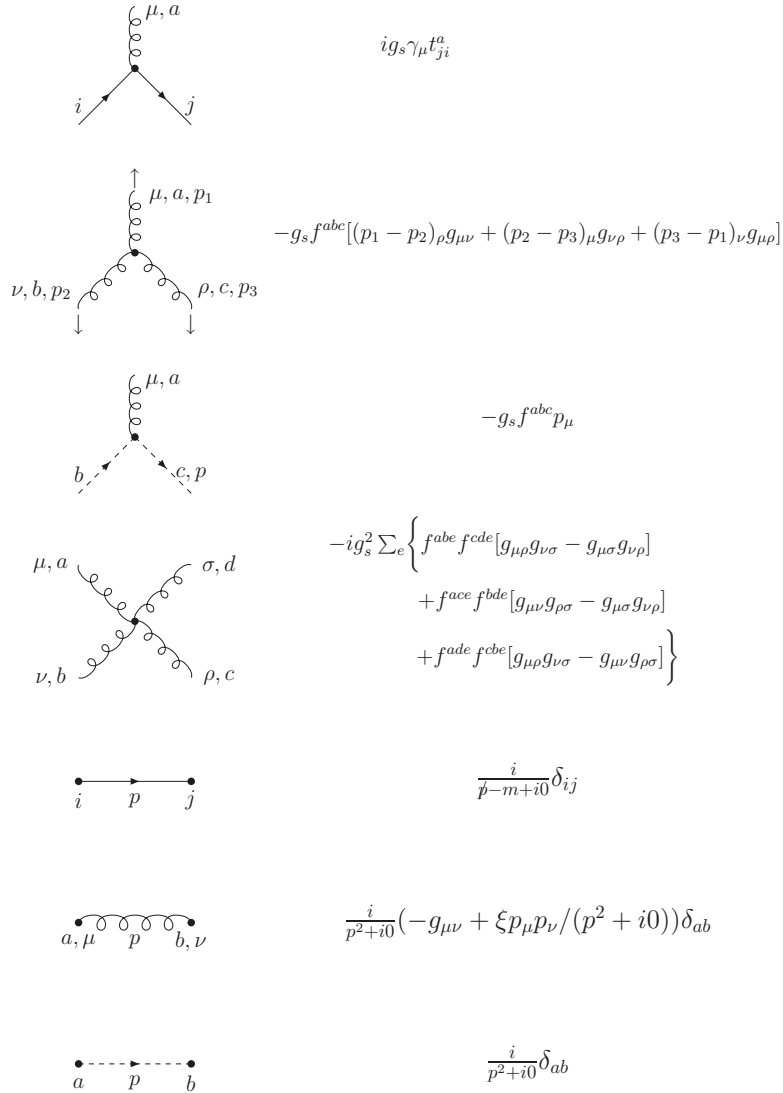


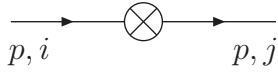
Figure B.1.: Feynman rules of QCD. Taken from [70].

## B. Feynman Rules

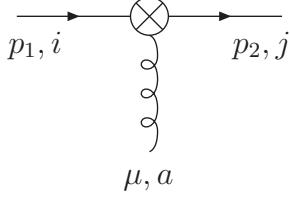
The Feynman rules for an operator insertion on a quark can be found in Figure B.2 while the insertion on a gluon requires the rules given in Figure B.3. They are taken from [182]. The terms  $\gamma_{\pm}$  differentiate between the unpolarized (+) and polarized (−) case. Gluon momenta have to be considered as incoming and  $\Delta$  is a light-like vector, i.e.  $\Delta^2 = 0$ . For the gluonic Feynman rules we follow Ref. [155]. However, one of them has to be corrected. The operator with four external legs has to read

$$O_{abcd}^{\mu\nu\rho\sigma}(p_1, p_2, p_3, p_4) = ig^2[1 - (-1)^N][f_{abe}f_{cde}O^{\mu\nu\rho\sigma}(p_1, p_2, p_3, p_4) + f_{ace}f_{bde}O^{\mu\rho\nu\sigma}(p_1, p_3, p_2, p_4) - f_{ade}f_{bce}O^{\rho\nu\mu\sigma}(p_3, p_2, p_1, p_4)]$$

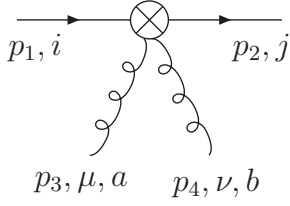
$$\begin{aligned} O^{\mu\nu\rho\sigma}(p_1, p_2, p_3, p_4) &= (\varepsilon^{\Delta\nu\rho\sigma}\Delta^\mu - \varepsilon^{\Delta\mu\rho\sigma}\Delta^\nu)[\Delta.p_3 + \Delta.p_4]^{N-2} \\ &\quad - \Delta^\rho(\varepsilon^{\nu\sigma\Delta p_4}\Delta^\mu - \varepsilon^{\mu\sigma\Delta s}\Delta^\nu) \sum_{i=1}^{N-3} [\Delta.p_3 + \Delta.p_4]^i (\Delta.p_4)^{N-i-3} \\ &\quad + \Delta^\sigma(\varepsilon^{\rho\nu\tau\Delta}\Delta^\mu - \varepsilon^{\rho\mu p_3\Delta}\Delta^\nu) \sum_{i=0}^{N-3} [\Delta.p_3 + \Delta.p_4]^{N-i-3} (\Delta.p_3)^i \\ &\quad - \Delta^\nu(\varepsilon^{\mu\sigma\Delta p_1}\Delta^\rho - \varepsilon^{\mu\rho\Delta p_1}\Delta^\sigma) \sum_{i=0}^{N-3} [\Delta.p_3 + \Delta.p_4]^{N-i-3} (-\Delta.p_1)^i \\ &\quad + \Delta^\mu(\varepsilon^{\nu\sigma\Delta p_2}\Delta^\rho - \varepsilon^{\nu\rho\Delta p_2}\Delta^\sigma) \sum_{i=0}^{N-3} [\Delta.p_3 + \Delta.p_4]^{N-i-3} (-\Delta.p_2)^i \\ &\quad + \Delta^\nu\Delta^\rho(\varepsilon^{\Delta\sigma p_1 p_4}\Delta^\mu + \varepsilon^{\mu\sigma\Delta p_4}\Delta.p_1) \sum_{j=0}^{N-4} \sum_{i=0}^j (\Delta.p_1)^{N-j-4} [\Delta.p_1 + \Delta.p_2]^{j-i} (-\Delta.p_4)^i \\ &\quad - \Delta^\mu\Delta^\rho(\varepsilon^{\Delta\sigma p_2 p_4}\Delta^\nu + \varepsilon^{\nu\sigma\Delta p_4}\Delta.p_2) \sum_{j=0}^{N-4} \sum_{i=0}^j (\Delta.p_2)^{N-j-4} [\Delta.p_1 + \Delta.p_2]^{j-i} (-\Delta.p_4)^i \\ &\quad - \Delta^\nu\Delta^\sigma(\varepsilon^{\Delta\mu p_1 p_3}\Delta^\rho + \varepsilon^{\mu\rho\Delta p_1}\Delta.p_3) \sum_{j=0}^{N-4} \sum_{i=0}^j (\Delta.p)^{N-j-4} [\Delta.p + \Delta.p_2]^{j-i} (-\Delta.r)^i \\ &\quad + \Delta^\mu\Delta^\sigma(\varepsilon^{\Delta\nu p_2 p_3}\Delta^\rho + \varepsilon^{\nu\rho\Delta p_1}\Delta.p_3) \sum_{j=0}^{N-4} \sum_{i=0}^j (\Delta.p_2)^{N-j-4} (\Delta.p_1 + \Delta.p_2)^{j-i} (-\Delta.p_3)^i. \end{aligned} \tag{B.1}$$



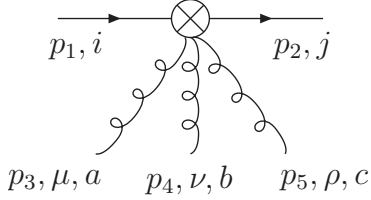
$$\delta^{ij} \not{\Delta} \gamma_{\pm} (\Delta \cdot p)^{N-1}, \quad N \geq 1$$



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



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



$$g^3 \Delta^\mu \Delta^\nu \Delta^\rho \not{\Delta} \gamma_{\pm} \sum_{j=0}^{N-4} \sum_{l=j+1}^{N-3} \sum_{m=l+1}^{N-2} (\Delta \cdot p_2)^j (\Delta \cdot p_1)^{N-m-2} \\ \left[ (t^a t^b t^c)_{ji} (\Delta \cdot p_4 + \Delta \cdot p_5 + \Delta \cdot p_1)^{l-j-1} (\Delta \cdot p_5 + \Delta \cdot p_1)^{m-l-1} \right. \\ + (t^a t^c t^b)_{ji} (\Delta \cdot p_4 + \Delta \cdot p_5 + \Delta \cdot p_1)^{l-j-1} (\Delta \cdot p_4 + \Delta \cdot p_1)^{m-l-1} \\ + (t^b t^a t^c)_{ji} (\Delta \cdot p_3 + \Delta \cdot p_5 + \Delta \cdot p_1)^{l-j-1} (\Delta \cdot p_5 + \Delta \cdot p_1)^{m-l-1} \\ + (t^b t^c t^a)_{ji} (\Delta \cdot p_3 + \Delta \cdot p_5 + \Delta \cdot p_1)^{l-j-1} (\Delta \cdot p_3 + \Delta \cdot p_1)^{m-l-1} \\ + (t^c t^a t^b)_{ji} (\Delta \cdot p_3 + \Delta \cdot p_4 + \Delta \cdot p_1)^{l-j-1} (\Delta \cdot p_4 + \Delta \cdot p_1)^{m-l-1} \\ \left. + (t^c t^b t^a)_{ji} (\Delta \cdot p_3 + \Delta \cdot p_4 + \Delta \cdot p_1)^{l-j-1} (\Delta \cdot p_3 + \Delta \cdot p_1)^{m-l-1} \right], \\ N \geq 4$$

$\gamma_+ = 1$ ,  $\gamma_- = \gamma_5$ . For transversity, one has to replace:  $\not{\Delta} \gamma_{\pm} \rightarrow \sigma^{\mu\nu} \Delta_\nu$ .

Figure B.2.: Feynman rules for quarkonic composite operators, taken from [182].

B. Feynman Rules

$$\begin{aligned}
& \text{Diagram 1: } \text{---} p, \nu, b \text{---} \otimes \text{---} p, \mu, a \text{---} \\
& \qquad \qquad \qquad \frac{1+(-1)^N}{2} \delta^{ab} (\Delta \cdot p)^{N-2} \\
& \qquad \qquad \qquad \left[ g_{\mu\nu} (\Delta \cdot p)^2 - (\Delta_\mu p_\nu + \Delta_\nu p_\mu) \Delta \cdot p + p^2 \Delta_\mu \Delta_\nu \right], \quad N \geq 2
\end{aligned}$$

$$\begin{aligned}
& \text{Diagram 2: } \begin{array}{c} \text{---} p_1, \mu, a \text{---} \otimes \text{---} p_3, \lambda, c \text{---} \\ \uparrow \\ p_2, \nu, b \end{array} \\
& \qquad \qquad \qquad -ig \frac{1+(-1)^N}{2} f^{abc} \left( \right. \\
& \qquad \qquad \qquad \left. \left[ (\Delta_\nu g_{\lambda\mu} - \Delta_\lambda g_{\mu\nu}) \Delta \cdot p_1 + \Delta_\mu (p_{1,\nu} \Delta_\lambda - p_{1,\lambda} \Delta_\nu) \right] (\Delta \cdot p_1)^{N-2} \right. \\
& \qquad \qquad \qquad \left. + \Delta_\lambda \left[ \Delta \cdot p_1 p_{2,\mu} \Delta_\nu + \Delta \cdot p_2 p_{1,\nu} \Delta_\mu - \Delta \cdot p_1 \Delta \cdot p_2 g_{\mu\nu} - p_1 \cdot p_2 \Delta_\mu \Delta_\nu \right] \right. \\
& \qquad \qquad \qquad \left. \times \sum_{j=0}^{N-3} (-\Delta \cdot p_1)^j (\Delta \cdot p_2)^{N-3-j} \right. \\
& \qquad \qquad \qquad \left. + \left\{ \begin{array}{c} p_1 \rightarrow p_2 \rightarrow p_3 \rightarrow p_1 \\ \mu \rightarrow \nu \rightarrow \lambda \rightarrow \mu \end{array} \right\} + \left\{ \begin{array}{c} p_1 \rightarrow p_3 \rightarrow p_2 \rightarrow p_1 \\ \mu \rightarrow \lambda \rightarrow \nu \rightarrow \mu \end{array} \right\} \right), \quad N \geq 2
\end{aligned}$$

$$\begin{aligned}
& \text{Diagram 3: } \begin{array}{c} \text{---} p_1, \mu, a \text{---} \otimes \text{---} p_4, \sigma, d \text{---} \\ \uparrow \qquad \uparrow \\ p_2, \nu, b \qquad p_3, \lambda, c \end{array} \\
& \qquad \qquad \qquad g^2 \frac{1+(-1)^N}{2} \left( f^{abe} f^{cde} O_{\mu\nu\lambda\sigma}(p_1, p_2, p_3, p_4) \right. \\
& \qquad \qquad \qquad \left. + f^{ace} f^{bde} O_{\mu\lambda\nu\sigma}(p_1, p_3, p_2, p_4) + f^{ade} f^{bce} O_{\mu\sigma\nu\lambda}(p_1, p_4, p_2, p_3) \right), \\
& \qquad \qquad \qquad O_{\mu\nu\lambda\sigma}(p_1, p_2, p_3, p_4) = \Delta_\nu \Delta_\lambda \left\{ -g_{\mu\sigma} (\Delta \cdot p_3 + \Delta \cdot p_4)^{N-2} \right. \\
& \qquad \qquad \qquad \left. + [p_{4,\mu} \Delta_\sigma - \Delta \cdot p_4 g_{\mu\sigma}] \sum_{i=0}^{N-3} (\Delta \cdot p_3 + \Delta \cdot p_4)^i (\Delta \cdot p_4)^{N-3-i} \right. \\
& \qquad \qquad \qquad \left. - [p_{1,\sigma} \Delta_\mu - \Delta \cdot p_1 g_{\mu\sigma}] \sum_{i=0}^{N-3} (-\Delta \cdot p_1)^i (\Delta \cdot p_3 + \Delta \cdot p_4)^{N-3-i} \right. \\
& \qquad \qquad \qquad \left. + [\Delta \cdot p_1 \Delta \cdot p_4 g_{\mu\sigma} + p_1 \cdot p_4 \Delta_\mu \Delta_\sigma - \Delta \cdot p_4 p_{1,\sigma} \Delta_\mu - \Delta \cdot p_1 p_{4,\mu} \Delta_\sigma] \right. \\
& \qquad \qquad \qquad \left. \times \sum_{i=0}^{N-4} \sum_{j=0}^i (-\Delta \cdot p_1)^{N-4-i} (\Delta \cdot p_3 + \Delta \cdot p_4)^{i-j} (\Delta \cdot p_4)^j \right\} \\
& \qquad \qquad \qquad - \left\{ \begin{array}{c} p_1 \leftrightarrow p_2 \\ \mu \leftrightarrow \nu \end{array} \right\} - \left\{ \begin{array}{c} p_3 \leftrightarrow p_4 \\ \lambda \leftrightarrow \sigma \end{array} \right\} + \left\{ \begin{array}{c} p_1 \leftrightarrow p_2, p_3 \leftrightarrow p_4 \\ \mu \leftrightarrow \nu, \lambda \leftrightarrow \sigma \end{array} \right\}, \quad N \geq 2
\end{aligned}$$

Figure B.3.: Feynman rules for gluonic composite operators in the unpolarized case, taken from [182].

## C. Special Functions

For the calculations in the main part of this thesis a large amount of special functions are used to express intermediate steps and the results. In this Appendix these quantities are defined and their algebraic properties are summarized. Many of these can be found in Ref. [432, 433].

### C.1. Euler's $\Gamma$ -function

Euler's  $\Gamma$ -function can be defined via the integral

$$\Gamma(z) = \int_0^{\infty} dt \exp(-t)t^{z-1}, \quad (\text{C.1})$$

for  $\text{Re}(z) > 0$ . From this representation it is easy to show, that

$$\Gamma(z+1) = z\Gamma(z). \quad (\text{C.2})$$

Equation (C.2) can be used to analytically continue the  $\Gamma$ -function and shows that the  $\Gamma$ -function itself is the analytic continuation of the factorial.

The  $\Gamma$ -function has no roots on the whole complex plane and only possesses simple poles at the non-positive integers. Their residue are given by

$$\text{Res}[\Gamma(z)]_{z=-k} = \frac{(-1)^k}{k!}, \quad k \in \mathcal{N}^0. \quad (\text{C.3})$$

The series expansion around  $z = 1$  is given by

$$\Gamma\left(1 - \frac{\varepsilon}{2}\right) = \exp\left(\frac{\varepsilon\gamma_E}{2}\right) \exp\left(\sum_{i=2}^{\infty} \frac{\zeta_i}{i} \left(\frac{\varepsilon}{2}\right)^i\right). \quad (\text{C.4})$$

Here  $\gamma_E$  is the Euler-Mascheroni constant, cf. (C.5), and  $\zeta_k$  are Riemann's  $\zeta$ -values. These constants are defined by

$$\gamma_E = \lim_{n \rightarrow \infty} \left( \sum_{k=1}^n \frac{1}{k} - \ln(n) \right), \quad (\text{C.5})$$

$$\zeta_k = \sum_{i=1}^{\infty} \frac{1}{i^k}, \quad k \geq 2, \quad k \in \mathbb{N}. \quad (\text{C.6})$$

The even  $\zeta$ -values can be expressed in terms of  $\pi$

$$\zeta_{2k} = \eta_k \pi^{2k} \quad (\text{C.7})$$

with

$$\eta_1 = \frac{1}{6}, \quad \eta_k = \sum_{l=1}^{k-1} (-1)^{l-1} \frac{\eta_{k-l}}{(2l+1)!} + (-1)^{k+1} \frac{k}{(2k+1)!} \quad (\text{C.8})$$

and are therefore not independent. The definition can be extended to multiple  $\zeta$ -values, if one considers the limit  $N \rightarrow \infty$  of harmonic sums. A reduction of multiple  $\zeta$ -values to a basis of algebraically independent ones up to weight 22 for non-alternating and weight 12 for alternating sums can be found in [434]. Furthermore, Euler's reflection

$$\Gamma(s - k) = (-1)^{k-1} \frac{\Gamma(-s)\Gamma(s + 1)}{\Gamma(k + 1 - s)}, \quad (\text{C.9})$$

for  $k \in \mathbb{N}$ ,  $s \notin \mathbb{Z}$  and Legendre's doubling

$$\Gamma(s + 2k) = \frac{(-1)^{1-s-2k}}{\pi} \Gamma\left(k + \frac{s}{2}\right) \Gamma\left(k + \frac{s}{2} + \frac{1}{2}\right) \quad (\text{C.10})$$

relation are frequently used in order to resolve pole structures of expressions involving  $\Gamma$ -functions or arriving at forward running sums. A closely related function is the Beta-function. For  $\text{Re}(\alpha), \text{Re}(\beta) > 0$  it has the following integral representation

$$B(\alpha, \beta) = \int_0^1 dx x^{\alpha-1} (1-x)^{\beta-1}. \quad (\text{C.11})$$

The integral evaluates to

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)}, \quad (\text{C.12})$$

which in turn can be used to analytically continue outside of the respective singularities.

An often used shorthand notation for rational functions of  $\Gamma$ -functions which will also be employed in this thesis is given by

$$\Gamma \left[ \begin{matrix} a_1^{b_1}, \dots, a_i^{b_i} \\ c_1^{d_1}, \dots, c_j^{d_j} \end{matrix} \right] = \frac{\Gamma^{b_1}(a_1) \dots \Gamma^{b_i}(a_i)}{\Gamma^{d_1}(c_1) \dots \Gamma^{d_j}(c_j)}. \quad (\text{C.13})$$

## C.2. Generalized Hypergeometric Functions

Another class of useful functions are the generalized hypergeometric functions  ${}_pF_Q$  [194, 195]. Here in particular the functions

$${}_{p+1}F_p \left[ \begin{matrix} a_1, \dots, a_{p+1} \\ b_1, \dots, b_p \end{matrix}; z \right] = \sum_{n=0}^{\infty} \frac{(a_1)_n \dots (a_{p+1})_n}{(b_1)_n \dots (b_p)_n} \frac{z^n}{\Gamma(n+1)} \quad (\text{C.14})$$

are of special interest. The Pochhammer symbol  $(a)_n$  is defined by

$$(a)_n = a(a+1) \dots (a+n-1), \quad (\text{C.15})$$

$$(a)_0 = 1. \quad (\text{C.16})$$

For  $a \in \mathcal{C}$  it can be written as

$$(a)_n = \frac{\Gamma(x+n)}{\Gamma(x)}. \quad (\text{C.17})$$

The series converges if either  $|z| < 1$  or  $|z| = 0$  and additionally

$$\text{Re} \left( \sum_{i=1}^p b_i - \sum_{i=1}^{p+1} a_i \right) > 0. \quad (\text{C.18})$$



However, there exist a plethora of contiguous and argument relations which allow for the analytic continuation. There exist even an integral representation, which is given recursively by

$${}_{p+1}F_p \left[ \begin{matrix} a_1, \dots, a_{p+1} \\ b_1, \dots, b_p \end{matrix}; z \right] = \frac{1}{B(a_{p+1}, b_p - a_{p+1})} \int_0^1 dx x^{a_{p+1}-1} (1-x)^{b_p - a_{p+1} - 1} {}_pF_{p-1} \left[ \begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_{p-1} \end{matrix}; xz \right] \quad (\text{C.19})$$

The recursion ends with the  ${}_2F_1$  for which we have

$${}_2F_1 \left[ \begin{matrix} a, b \\ c \end{matrix}; z \right] = \frac{1}{B(b, c-b)} \int_0^1 dx x^{b-1} (1-x)^{c-b-1} (1-xz)^{-a} \quad (\text{C.20})$$

Since the  ${}_2F_1$  has some particularly nice features, we want to list some in the following. With the argument transformations  $z \rightarrow 1-z$  and  $z \rightarrow \frac{z}{z-1}$  we can analytically continue  ${}_2F_1$  and arrive at convergent sum representations even if the initial representation would not allow for this. The relations are given by

$${}_2F_1 \left[ \begin{matrix} a, b \\ c \end{matrix}; z \right] = (1-z)^{-a} {}_2F_1 \left[ \begin{matrix} a, c-b \\ c \end{matrix}; \frac{z}{z-1} \right], \quad (\text{C.21})$$

$${}_2F_1 \left[ \begin{matrix} a, b \\ c \end{matrix}; z \right] = \Gamma \left[ \begin{matrix} c, c-a-b \\ c-a, c-b \end{matrix} \right] {}_2F_1 \left[ \begin{matrix} a, b \\ a+b-c+1 \end{matrix}; 1-z \right] \quad (\text{C.22})$$

$$+ (1-z)^{c-a-b} \Gamma \left[ \begin{matrix} c, a+b-c \\ a, b \end{matrix} \right] {}_2F_1 \left[ \begin{matrix} c-a, c-b \\ c-a-b+1 \end{matrix}; 1-z \right]. \quad (\text{C.23})$$

Furthermore, it is possible to find a closed form solution for  $z = 1$  and  $\text{Re}(c-a-b) > 0$  which is known as Gauß's theorem

$${}_2F_1 \left[ \begin{matrix} a, b \\ c \end{matrix}; 1 \right] = \Gamma \left[ \begin{matrix} c, c-a-b \\ c-a, c-b \end{matrix} \right]. \quad (\text{C.24})$$

Another useful representation of the  ${}_2F_1$  is the complex contour integral

$${}_2F_1 \left[ \begin{matrix} a, b \\ c \end{matrix}; z \right] = \frac{1}{2\pi i} \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \int_{-i\infty}^{+i\infty} d\sigma \frac{\Gamma(a+\sigma)\Gamma(b+\sigma)\Gamma(-\sigma)}{\Gamma(c+\sigma)} (-z)^\sigma, \quad (\text{C.25})$$

where the contour has to be chosen such that it separates the left-going poles, i.e. the poles from  $\Gamma(a+\sigma)$  and  $\Gamma(b+\sigma)$ , from the right-going poles, i.e. the poles from  $\Gamma(-\sigma)$ . It can be used to proof the identity

$$\frac{1}{(A+B)^\lambda} = \frac{1}{2\pi i} \int_{-i\infty}^{+i\infty} d\sigma \frac{\Gamma(-\sigma)\Gamma(\lambda+\sigma)}{\Gamma(\lambda)} \frac{A^\sigma}{B^{\lambda+\sigma}}, \quad (\text{C.26})$$

by identifying  $a = \lambda$ ,  $b = c$  and  $z = -A/B$ . Equation (C.26) can be used to split complicated Feynman-parameter polynomials raised to real powers by introducing a complex contour integral, also called Mellin-Barnes integral [188–191]. In the calculation of two mass effects for the OMEs it is frequently used to separate the two masses.

### C.3. Nested Sums

As it turns out the result of the OMEs for general values of the Mellin variable  $N$  is best described by nested sums. These sums have the general form

$$\sum_{i_1=1}^N a_1(i_1) \sum_{i_2=1}^{i_1} a_2(i_2) \cdots \sum_{i_k=1}^{i_{k-1}} a_k(i_k). \quad (\text{C.27})$$

The value of  $k$  is called the nesting depth. The first class of these sums encountered in computations in QFTs are the harmonic sums, cf. [149, 150]. They can be defined recursively as

$$S_{n_1, \dots, n_k}(N) = \sum_{i=1}^N \frac{(\text{sign}(n_1))^i}{i^{|n_1|}} S_{n_2, \dots, n_k}(i). \quad (\text{C.28})$$

The  $n_j$  are not allowed to be zero and the sum of their absolute values  $w = |n_1| + \dots + |n_k|$  defines the weight of the sum. A simple generalization of harmonic sums can be achieved by allowing for additional weights. The generalized harmonic sums [240, 250] are accordingly defined via

$$S_{n_1, \dots, n_k}(x_1, \dots, x_k; N) = \sum_{i=1}^N \frac{x_1^i}{i^{|n_1|}} S_{n_2, \dots, n_k}(i), \quad (\text{C.29})$$

with non-negative integers  $n_j$  and non-zero real parameters  $x_j$ . The harmonic sums emerge as special cases for  $x_j \in \{-1, 1\}$ . In further calculations also cyclotomic harmonic sums [275]

$$S_{\{a_1, b_1, c_1\}, \dots, \{a_k, b_k, c_k\}}(x_1, \dots, x_k; N) = \sum_{i=0}^N \frac{x_1^i}{(a_1 i + b_1)^{c_1}} S_{\{a_1, b_1, c_1\}, \dots, \{a_k, b_k, c_k\}}(x_2, \dots, x_k; N), \quad (\text{C.30})$$

with  $a_j, c_j \in \mathcal{N}$  and  $b_j \in \mathcal{N}^0$  and binomially weighted sums [241, 435–437], where summands of the form

$$\binom{2n}{n} \frac{x_j^n}{n^{m_j}} \quad (\text{C.31})$$

with  $b_j = \{-1, 0, +1\}$  contribute. We will not introduce a separate notation for the binomially weighted sums but write them out explicitly.

A very important algebraic property of nested sums is the stuffle or quasi-shuffle algebra [149, 150, 286, 438, 439]. It arises from the splitting of the direct product of two nested sums

$$\left( \sum_{i=1}^N a_i \right) \left( \sum_{i=1}^N b_i \right) = \sum_{i=1}^N a_i \sum_{j=1}^i b_j + \sum_{j=1}^N b_j \sum_{i=1}^j a_i - \sum_{i=1}^N a_i b_i. \quad (\text{C.32})$$

The relations can be applied iteratively to reduce sums of a given weight to a smaller set of so called basis sums [438, 439].

### C.4. Iterated Integrals

The nested sums introduced in Appendix C.3 are closely related to iterated integrals through Mellin-transforms. They have the general form

$$G(\{a_1, \dots, a_k\}, x) = \int_0^x d\tau_1 a_1(\tau_1) \int_0^{\tau_1} d\tau_2 a_2(\tau_2) \cdots \int_0^{\tau_{k-1}} d\tau_k a_k(\tau_k) \quad (\text{C.33})$$

and special classes of functions emerge from restricting the letters  $a_j$  to a restricted set of possibilities. The set  $\mathcal{A}$  is called the alphabet. The alphabet

$$\mathcal{A} = \left\{ f_1(x) = \frac{1}{1-x}, f_0(x) = \frac{1}{x}, f_1(x) = \frac{1}{1+x} \right\} \quad (\text{C.34})$$

leads to the harmonic polylogarithms (HPLs) [151] with the notation

$$\begin{aligned} H_{\underbrace{0, \dots, 0}_{k \text{ times}}}(x) &= \frac{1}{k!} \ln^k(x), \\ H_m(x) &= \int_0^x d\tau f_m(\tau), \quad x \neq 0, \\ H_{m_1, \dots, m_k}(x) &= \int_0^x d\tau f_{m_1}(\tau) H_{m_2, \dots, m_k}(\tau). \end{aligned} \quad (\text{C.35})$$

In this thesis we will use both notations, the one given in (C.33) with explicitly given letters and the one given in (C.35) where we have to introduce new letters in order to represent our new results of massive phase space integrals. The notation in (C.35) is especially suited to compactify results. The number of integrations  $k$  is called the weight of the function. The class of HPLs has the classical polylogarithms [264, 266]

$$\text{Li}_n(x) = H_{\underbrace{0, \dots, 0}_{n-1 \text{ times}}, 1}(x) \quad (\text{C.36})$$

and Nielsen-integrals [264, 440–442]

$$S_{n,p}(x) = \frac{(-1)^{n+p-1}}{(n-1)!p!} \int_0^1 \frac{dz}{z} \ln^{n-1}(z) \ln^p(1-xz) = H_{\underbrace{0, \dots, 0}_{n \text{ times}}, \underbrace{1, \dots, 1}_{p \text{ times}}}(x) \quad (\text{C.37})$$

as subsets. HPLs are related to harmonic sums introduced in Equation (C.28) through the Mellin-transform and appear in the expansions of HPLs around the argument  $x = 0$ . In order to be able to express all harmonic sums as Mellin transforms of HPLs one has to introduce  $+$ -distributions  $[f(x)]_+$ . They are defined through the integral relation

$$\int_0^1 dx [f(x)]_+ g(x) = \int_0^1 dx f(x) (g(x) - g(1)). \quad (\text{C.38})$$

In this way it is for example possible to express the harmonic sum  $S_1(N)$  as

$$S_1(N) = \int_0^1 dx \frac{x^N - 1}{x - 1}. \quad (\text{C.39})$$

To express  $N$ -independent constants in  $x$ -space it is also necessary to introduce  $\delta$ -distributions.

The generalization of HPLs which leads to the cyclotomic sums are called cyclotomic polylogarithms [275] and are based on the cyclotomic polynomials  $\Phi_n(x)$  [443]

$$\Phi_n(x) = \prod_{\substack{1 \leq k \leq n \\ \gcd(k,n)=1}} \left[ x - \exp\left(2\pi i \frac{k}{n}\right) \right]. \quad (\text{C.40})$$

### C. Special Functions

Based on these the alphabet of the cyclotomic HPLs is given by

$$\mathcal{A} = \left\{ f_0(x) = \frac{1}{x} \right\} \cup \left\{ f_{(n;b)} = \frac{x^b}{\Phi_n(x)} \mid n \in \mathcal{N}, b \in \mathcal{N}^0, b < \varphi(n) \right\}, \quad (\text{C.41})$$

where  $\varphi$  denotes Eulers totient function. Cyclotomic HPLs are closely related to Goncharov polylogarithms, where the cyclotomic polynomials are factored over the imaginary numbers and reduced to linear polynomials in the denominator. The Cyclotomic ones are advantageous since they are completely real representations and avoid spurious imaginary parts and a intermediate swell of the number of needed functions.

The binomially weighted sums, cf. Equation (C.31), are closely related to square root valued letters [241]. For this class of functions we do not introduce a special notation but refer to the notation of Equation (C.33) with explicitly written letters.

Analogously to the stuffle relations of nested sums, iterated integrals fulfill shuffle relations, which are also based on the multiplication of two iterated integrals and slicing the integration bounds. The simplest case is given by

$$\int_0^x dy f(y) \int_0^x dz g(z) = \int_0^x dy f(y) \int_0^y dz g(z) + \int_0^x dz g(z) \int_0^z dy f(y). \quad (\text{C.42})$$

Iteratively applying these relations can be used to reduce iterated integrals of a specific weight to a smaller basis of independent basis functions. For HPLs up to weight 6 these relations can be found in [438, 439].

# D. Pure-Singlet Heavy Flavor Wilson Coefficients at NLO – Computational Details

Our calculation closely follows classical calculations in the literature, cf. e.g. [131, 421, 444, 445]. Although these calculations are typically well documented, we encountered subtleties at several points of our calculation. Therefore, we provide a more detailed discussion of our calculation in the massless and massive case in this Appendix. First we will give the parametrization of the phase space we used in the massless and massive case, then we will proceed by explaining the angular integration and give explicit results for the angular integrals in  $d$  dimensions. In the end, we will comment on our resolution of the poles in  $\varepsilon$  and subtleties encountered in the massless case.

## D.1. Phase Space Parametrization

### The $2 \rightarrow 2$ Process

In the  $2 \rightarrow 2$  case in Figure 3.1 we refer to the invariants

$$s = (q + p)^2, \quad t = (q - k_1)^2, \quad u = (q - k_2)^2 \quad (\text{D.1})$$

with

$$s + t + u = -Q^2 + 2m^2 \quad \text{and} \quad Q^2 = -q^2. \quad (\text{D.2})$$

We will also use the notation  $\beta = \sqrt{1 - 4m^2/s}$ . In the centre-of-mass system of the outgoing particles,  $\vec{k}_1 + \vec{k}_2 = 0$ , the scattering angle  $\theta$  is defined by

$$t = -Q^2 + m^2 - 2q^0 k_1^0 + |\vec{k}_1| |\vec{q}| \cos(\theta) = m^2 - \frac{Q^2}{2x} (1 - \beta \cos(\theta)), \quad (\text{D.3})$$

with

$$q^0 = \frac{s - Q^2}{2\sqrt{s}}, \quad |\vec{q}| = \frac{s - Q^2}{2\sqrt{s}}, \quad (\text{D.4})$$

$$k_1^0 = \frac{\sqrt{s}}{2}, \quad |\vec{k}_1| = \frac{\sqrt{s}}{2} \beta \quad (\text{D.5})$$

and

$$\lambda(a, b, c) = (a - b - c)^2 - 4bc. \quad (\text{D.6})$$

The phase space integral is given by

$$\int d\text{PS}_2 = 2^{4-2d} \frac{\pi^{1-d/2}}{\Gamma(\frac{d}{2} - 1)} s^{d/2-2} \beta^{d-3} \int_0^\pi d\theta \sin^{d-3}(\theta). \quad (\text{D.7})$$

The limit  $m \rightarrow 0$  is easily obtained by setting  $m = 0$  and  $\beta = 1$ .

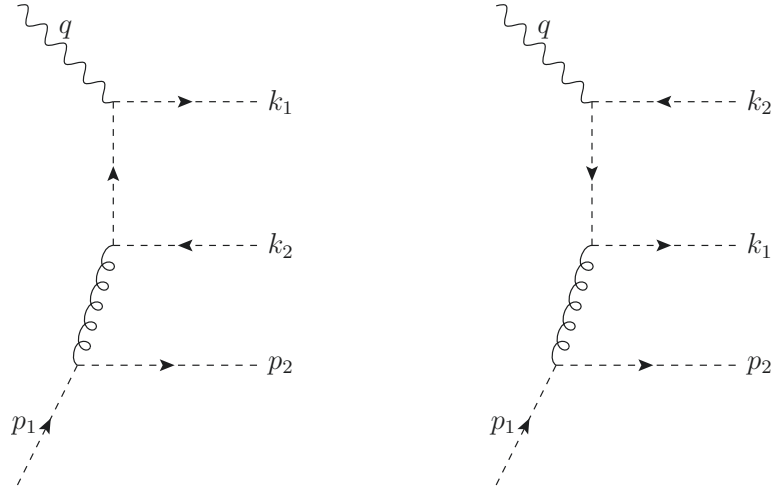


Figure D.1.: Diagrams of the  $O(a_s^2)$  contributions to the pure singlet scattering cross section  $\gamma^* + q \rightarrow Q + \bar{Q} + q$ .

### The $2 \rightarrow 3$ Process

The  $2 \rightarrow 3$  process is slightly more involved. The contributing Feynman diagrams are shown in Figure D.1. We use

$$\begin{aligned}
 \int d\text{PS}_3 &= \int \frac{d^d p_2}{(2\pi)^{d-1}} \int \frac{d^d k_1}{(2\pi)^{d-1}} \int \frac{d^d k_2}{(2\pi)^{d-1}} \delta^+(p_2^2) \delta^+(k_1^2 - m^2) \delta^+(k_2^2 - m^2) \\
 &\times (2\pi)^d \delta^{(d)}(p_1 + q - p_2 - k_1 - k_2) \\
 &= \frac{1}{(2\pi)^{2d-3}} \int ds_{12} \left\{ \int d^d p_2 \int d^d K \delta^+(p_2^2) \delta^+(K^2 - s_{12}) \delta^{(d)}(p_1 + q - p_2 - K) \right\} \\
 &\times \left\{ \int d^d k_1 \int d^d k_2 \delta^+(k_1^2 - m^2) \delta^+(k_2^2 - m^2) \delta^{(d)}(k_1 + k_2 - K) \right\}. \quad (\text{D.8})
 \end{aligned}$$

Here

$$1 = \int ds_{12} \int d^d K \delta^+(K^2 - s_{12}) \delta^{(d)}(k_1 + k_2 - K) \quad (\text{D.9})$$

was introduced to factorize the  $2 \rightarrow 3$  phase space into a  $(2 \rightarrow 2) \times (1 \rightarrow 2)$  phase space. Both can now be calculated in the most appropriate system independent from each other. Integrating the first factor in the centre-of-mass system of the process and the second in the one of the two heavy quarks one obtains

$$\begin{aligned}
 \int d\text{PS}_3 &= \frac{1}{(4\pi)^d} \frac{(s - q^2)^{3-d}}{\Gamma(d-3)} \int_{s_{12}^-}^{s_{12}^+} ds_{12} \int_{t^-}^{t^+} dt \int_0^\pi d\theta \int_0^\pi d\phi [\sin(\theta)]^{d-3} [\sin(\phi)]^{d-4} \\
 &\times s_{12}^{d/2-2} \left[ 1 - \frac{4m^2}{s_{12}} \right]^{d/2-3/2} [(s - q^2)u - q^2 t]^{d/2-2} t^{d/2-2}, \quad (\text{D.10})
 \end{aligned}$$

where we have chosen the kinematic invariants

$$t = 2p_1 \cdot p_2, \quad u = 2p_2 \cdot q, \quad s = (p_1 + q)^2, \quad s_{12} = s - t - u. \quad (\text{D.11})$$

The phase space boundary is given by

$$s_{12}^- = 4m^2, \quad s_{12}^+ = s, \quad (\text{D.12})$$

$$t^- = 0, \quad t^+ = \frac{1}{s}(s - q^2)(s - s_{12}). \quad (\text{D.13})$$

We can use the following explicit parameterization of the vectors

$$k_1 = \left( k^0, 0, \dots, |\vec{k}| \sin(\phi) \sin(\theta), |\vec{k}| \cos(\phi) \sin(\theta), |\vec{k}| \cos(\theta) \right), \quad (\text{D.14})$$

$$k_2 = \left( k^0, 0, \dots, -|\vec{k}| \sin(\phi) \sin(\theta), -|\vec{k}| \cos(\phi) \sin(\theta), -|\vec{k}| \cos(\theta) \right), \quad (\text{D.15})$$

$$p_1 = \frac{s - t - q^2}{2\sqrt{s_{12}}} (1, \dots, 0, 0, 1), \quad (\text{D.16})$$

$$p_2 = \frac{s - s_{12}}{2\sqrt{s_{12}}} (1, 0, \dots, \sin(\chi), \cos(\chi)), \quad (\text{D.17})$$

$$q = \frac{1}{2\sqrt{s_{12}}} (q^2 + s_{12} + t, \dots, 0, 0, (s - s_{12}) \sin(\chi), q^2 + t - s + (s - s_{12}) \cos(\chi)), \quad (\text{D.18})$$

$$\cos(\chi) = 1 - \frac{2s_{12}t}{(s - t - q^2)(s - s_{12})}, \quad (\text{D.19})$$

$$k^0 = \frac{\sqrt{s_{12}}}{2}, \quad (\text{D.20})$$

$$|\vec{k}| = \frac{\sqrt{s_{12}}}{2} \sqrt{1 - \frac{4m^2}{s_{12}}}. \quad (\text{D.21})$$

In the limit  $m \rightarrow 0$ , we recover the parameterization given in [131].

In a next step we want to introduce dimensionless variables with support over the unit cube. Here it is advantageous to distinguish between the massless and the massive case. In the massless case, we follow [131] and introduce the new variables

$$\begin{aligned} z &= -\frac{q^2}{s - q^2}, \\ u &= [1 - z - y - (1 - z)(1 - y)x](s - q^2), \\ t &= y(s - q^2). \end{aligned} \quad (\text{D.22})$$

The massless three-particle phase space then reads

$$\begin{aligned} \int d\text{PS}_3(m=0) &= \frac{1}{(4\pi)^d} \frac{(s - q^2)^{3-d}}{\Gamma(d-3)} \int_0^\pi d\theta \int_0^\pi d\phi (\sin(\theta))^{d-3} (\sin(\phi))^{d-4} \\ &\times \int_0^{s-q^2} dt \int_{tq^2/(s-q^2)}^{s-t} du s_{12}^{d/2-2} t^{d/2-2} [(s - q^2)u - q^2t]^{d/2-2} \\ &= \frac{1}{(4\pi)^d} \frac{(s - q^2)^{3-d}}{\Gamma(d-3)} (1 - z)^{d-3} \int_0^\pi d\theta \int_0^\pi d\phi (\sin(\theta))^{d-3} (\sin(\phi))^{d-4} \\ &\times \int_0^1 dy \int_0^1 dx y^{d/2-2} (1 - y)^{d-3} [x(1 - x)]^{d/2-2}. \end{aligned} \quad (\text{D.23})$$

In the massive case the change to the following variables is useful

$$z = -\frac{q^2}{s - q^2},$$

$$\begin{aligned}
 x &= \frac{1}{\beta^2} \left( 1 - \frac{4m^2}{s_{12}} \right), & s_{12} &= \frac{4m^2}{1 - \beta^2 x}, \\
 y &= \frac{st}{(s - q^2)(s - s_{12})}, & t &= (s - q^2)\beta^2 y \frac{1 - x}{1 - \beta^2 x}.
 \end{aligned} \tag{D.24}$$

The new parameterization then reads

$$\begin{aligned}
 \int d\text{PS}_3 &= \frac{1}{(4\pi)^d} \frac{s^{d-3}}{\Gamma(3-d)} \beta^{3d-7} (1 - \beta^2)^{d/2-1} \int_0^1 dx \int_0^1 dy \int_0^\pi d\theta \int_0^\pi d\phi [\sin(\theta)]^{d-3} [\sin(\phi)]^{d-4} \\
 &\times y^{d/2-2} (1-y)^{d/2-2} x^{d/2-3/2} (1-x)^{d-3} (1-\beta^2 x)^{3-3d/2}.
 \end{aligned} \tag{D.25}$$

The limit  $m \rightarrow 0$  is not easily recovered, because of the mass dependent transformation.

## D.2. Angular Integrals

### The massless case

There are four angle dependent denominator structures appearing for the pure singlet process:

$$\begin{aligned}
 N_1 &= (p_1 - k_1)^2 = -2p_1 \cdot k_1 = a(1 - \cos(\theta)), \\
 N_2 &= (p_1 - k_2)^2 = -2p_1 \cdot k_2 = a(1 + \cos(\theta)), \\
 N_3 &= (q - k_1)^2 = q^2 - 2q \cdot k_1 = A + B \cos(\theta) + C \cos(\phi) \sin(\theta), \\
 N_4 &= (q - k_2)^2 = q^2 + 2q \cdot k_1 = A - B \cos(\theta) - C \cos(\phi) \sin(\theta),
 \end{aligned} \tag{D.26}$$

with

$$\begin{aligned}
 a &= -\frac{s - t - q^2}{2}, \\
 A &= \frac{1}{2} (q^2 - s_{12} - t), \\
 B &= \frac{1}{2} [q^2 - s + t + (s - s_{12}) \cos(\chi)], \\
 C &= \frac{s - s_{12}}{2} \sin(\chi).
 \end{aligned} \tag{D.27}$$

Using partial fractioning we can express all angular integrals via

$$I_{l,k} = \int_0^\pi d\theta \int_0^\pi d\phi \frac{\sin^{d-3}(\theta)}{a^l [1 - \cos(\theta)]^l} \frac{\sin^{d-4}(\phi)}{[A + B \cos(\theta) + C \sin(\theta) \cos(\phi)]^k}. \tag{D.28}$$

We only encounter integrals with  $k \leq 0$ , however, it is possible to find closed form solutions for  $k \leq 0$  and  $l \leq 0$  in the massless case. In the following we will list the result for these angular integrals in  $d$ -dimensions.

$l$  negative:

$$\begin{aligned}
 I_{l,k} &= \sum_{m=0}^k \sum_{n=0}^{-l-m} \binom{-l}{m} \binom{-k-m}{n} 2^{2d-7} a^{-l} (B^2 + C^2)^{l/2} \left( B + \sqrt{B^2 + C^2} \right)^{-l-m-n} \\
 &\times (-2B)^n \left( A - \sqrt{B^2 + C^2} \right)^{-k} (2C)^m \frac{\Gamma^2(d/2 - 3/2)}{\Gamma(d-3)} {}_2F_1 \left[ \begin{matrix} -m, d/2 - 3/2 \\ d-3 \end{matrix}, 2 \right]
 \end{aligned}$$



$$\times \frac{\Gamma(d/2 - 1 + n + m/2)\Gamma(d/2 - 1 + m/2)}{\Gamma(d - 2 + m + n)} {}_2F_1 \left[ \begin{matrix} k, d/2 - 1 + n + m/2 \\ d - 2 + m + n \end{matrix}, -\frac{2\sqrt{B^2 + C^2}}{A - \sqrt{B^2 + C^2}} \right].$$

For  $l = 0$  this reduces to

$$I_{0,k} = 2^{2d-7} \left[ A - \sqrt{B^2 + C^2} \right]^{-k} \frac{\Gamma^2(d/2 - 3/2)}{\Gamma(d - 3)} \frac{\Gamma^2(d/2 - 1)}{\Gamma(d - 2)} \times {}_2F_1 \left[ \begin{matrix} k, d/2 - 1 \\ d - 2 \end{matrix}, -\frac{2\sqrt{B^2 + C^2}}{A - \sqrt{B^2 + C^2}} \right]. \quad (\text{D.29})$$

$k$  negative:

$$I_{l,k} = \sum_{m=0}^{-k} \binom{-k}{m} \frac{2^{2d-7-l}}{a^l} (A - B)^{-k-m} (-2z)^m \frac{\Gamma^2(d/2 - 3/2)}{\Gamma(d - 3)} {}_2F_1 \left[ \begin{matrix} -m, d/2 - 3/2 \\ d - 3 \end{matrix}, 2 \right] \times \frac{\Gamma(d/2 - 1 + m/2)\Gamma(d/2 - 1 + m/2 - l)}{\Gamma(d - 2 + m - l)} {}_2F_1 \left[ \begin{matrix} m + k, d/2 - 1 + m/2 \\ d - 2 + m - l \end{matrix}, -\frac{2B}{A - B} \right].$$

For  $k = 0$  this reduces to

$$I_{l,0} = \frac{2^{2d-7-l}}{a^l} \frac{\Gamma(d/2 - 1 - l)\Gamma(d/2 - 1)}{\Gamma(d - 2 - l)} \frac{\Gamma^2(d/2 - 3/2)}{\Gamma(d - 3)}. \quad (\text{D.30})$$

Expanding these results around  $\varepsilon = d - 4$  dimensions we recover the integrals given in [444].

### The massive case

In the massive case the four denominator structures read

$$\begin{aligned} N_1 &= (p_1 - k_1)^2 = -2p_1 \cdot k_1 = a + b \cos(\theta), \\ N_2 &= (p_1 - k_2)^2 = -2p_1 \cdot k_2 = a - b \cos(\theta), \\ N_3 &= (q - k_1)^2 = q^2 - 2q \cdot k_1 = A + B \cos(\theta) + C \cos(\phi) \sin(\theta) \\ N_4 &= (q - k_2)^2 = q^2 - 2q \cdot k_2 = A - B \cos(\theta) - C \cos(\phi) \sin(\theta), \end{aligned} \quad (\text{D.31})$$

with

$$a = -\frac{s - t - q^2}{2}, \quad (\text{D.32})$$

$$b = -\frac{1}{2} \sqrt{1 - \frac{4m^2}{s_{12}}} (q_2 - s - t), \quad (\text{D.33})$$

$$A = \frac{q^2 - s_{12} - t}{2}, \quad (\text{D.34})$$

$$B = \frac{1}{2} \sqrt{1 - \frac{4m^2}{s_{12}}} (q^2 - s + t + (s - s_{12}) \cos(\chi)), \quad (\text{D.35})$$

$$C = \frac{1}{2} \sqrt{1 - \frac{4m^2}{s_{12}}} (s - s_{12}) \sin(\chi). \quad (\text{D.36})$$

Therefore, we have to consider the more general angular integral

$$I_{l,k} = \int_0^\pi d\theta \int_0^\pi d\phi \frac{\sin^{d-3}(\theta)}{[a + b \cos(\theta)]^l} \frac{\sin^{d-4}(\phi)}{[A + B \cos(\theta) + C \sin(\theta) \cos(\phi)]^k} \quad (\text{D.37})$$

in the following.

$l$  negative:

For  $l \leq 0$  and arbitrary  $k$  (the only case we encounter), we find:

$$\begin{aligned}
 I_{l,k} &= \sum_{n=0}^{-l} \sum_{m=0}^n \sum_{i=0}^m \binom{-l}{n} \binom{n}{m} \binom{m}{i} \left( \frac{bC}{\sqrt{B^2 + C^2}} \right)^{-l-n} a^{n-m} \left( \frac{bB}{\sqrt{B^2 + C^2}} \right)^m \left( A - \sqrt{B^2 + C^2} \right)^{-k} \\
 &\times 2^{2d-7-n-l+i} (-1)^{-n-l+m-i} \frac{\Gamma^2(d/2 - 3/2)}{\Gamma(d-3)} \\
 &\times \frac{\Gamma(d/2 - 1 - n/2 - l/2 + i) \Gamma(d/2 - 1 - n/2 - l/2)}{\Gamma(d-2-n-l+i)} \\
 &\times {}_2F_1 \left[ \begin{matrix} n+l, d/2 - 3/2 \\ d-3 \end{matrix}, 2 \right] {}_2F_1 \left[ \begin{matrix} k, d/2 - 1 - n/2 - l/2 + i \\ d-2-n-l+i \end{matrix}, -\frac{2\sqrt{B^2 + C^2}}{A - \sqrt{B^2 + C^2}} \right]. \tag{D.38}
 \end{aligned}$$

$k$  negative:

For  $k \leq 0$  and arbitrary  $l$ , we find:

$$\begin{aligned}
 I_{l,k} &= \sum_{m=0}^{-k} \sum_{n=0}^{-k-m} \binom{-k}{m} \binom{-k-m}{n} B^n C^m (a-b)^{-l} (A-B)^{-k-m-n} \\
 &\times (-1)^m 2^{m+n+1} \Gamma^2\left(\frac{1}{2}\right) \frac{\Gamma(n + \frac{m}{2} + 1) \Gamma(\frac{m}{2} + 1)}{\Gamma(m+n+2)} \\
 &\times {}_2F_1 \left[ \begin{matrix} -m, \frac{1}{2} \\ 1 \end{matrix}, 2 \right] {}_2F_1 \left[ \begin{matrix} l, n + \frac{m}{2} + 1 \\ m+n+2 \end{matrix}, -\frac{2b}{a-b} \right]. \tag{D.39}
 \end{aligned}$$

### D.3. Regularization

In order to perform the  $\varepsilon$ -expansion of the functions we use a simple subtraction term for  $y = 0$ . However, there is a subtlety hiding in this limit. The hypergeometric functions of interest are all of the argument

$$X = -\frac{2\sqrt{B^2 + C^2}}{A - \sqrt{B^2 + C^2}}. \tag{D.40}$$

Inserting the coefficients from Eqs. (D.27), we see that

$$X = 1 + \mathcal{O}(y), \tag{D.41}$$

which means that there is a potential logarithmic singularity for  $y \rightarrow 0$  in the massless case. This divergence can be made explicit by transforming the  ${}_2F_1$ 's from argument  $x$  to  $(1-x)$  [192–195]

$$\begin{aligned}
 {}_2F_1 \left[ \begin{matrix} a, b \\ c \end{matrix}, z \right] &= \Gamma \left[ \begin{matrix} c, c-a-b \\ c-a, c-b \end{matrix} \right] {}_2F_1 \left[ \begin{matrix} a, b \\ a+b-c+1 \end{matrix}, 1-z \right] \\
 &+ (1-z)^{c-a-b} \Gamma \left[ \begin{matrix} c, a+b-c \\ a, b \end{matrix} \right] {}_2F_1 \left[ \begin{matrix} c-a, c-b \\ c-a-b+1 \end{matrix}, 1-z \right]. \tag{D.42}
 \end{aligned}$$

The new hypergeometric functions have Taylor expansions around  $y = 0$ . The only singular behavior can now occur for  $y \rightarrow 0$ . This means that we can resolve the divergences via

$$F(x) = \int_0^1 dz \int_0^1 dy y^{-2+\varepsilon/2} f(x, y, z) \tag{D.43}$$

$$\begin{aligned}
 &= \int_0^1 dz \int_0^1 dy y^{-2+\varepsilon/2} \left[ f(x, y, z) - f^{(0)}(x, 0, z) - y f^{(1)}(x, 0, z) \right] \\
 &\quad - \int_0^1 dz \int_0^1 dy y^{-2+\varepsilon/2} \left[ f^{(0)}(x, 0, z) + y f^{(1)}(x, 0, z) \right] \\
 &\equiv (A) - (B),
 \end{aligned} \tag{D.44}$$

where we used the notation

$$f(x, y, z) = \sum_{i=0}^{\infty} y^i f^{(i)}(x, 0, z). \tag{D.45}$$

In the massive case we have

$$X = -\frac{\sqrt{B^2 + C^2}}{A - \sqrt{B^2 + C^2}} = \frac{2\beta\sqrt{z}}{1 + \beta\sqrt{z}} + \mathcal{O}(y), \tag{D.46}$$

which means that this divergence is regulated by the quark mass. The subtraction term ( $B$ ) can be trivially integrated over  $y$ , which will lead to poles in  $\varepsilon$ . In the massless case the expansion in  $\varepsilon$  can be performed afterwards and the last integration over  $z$  can be carried out. In the massive case there can be additional singularities hiding in the  $z \rightarrow 1$  limit. Therefore, term ( $B$ ) has to be regularized accordingly. Term ( $A$ ) is not singular in the limit  $y \rightarrow 0$  and can be expanded in  $\varepsilon$  and then integrated over  $y$  and  $z$ .

## D.4. Contributing expressions due to renormalization

In the following we list some Mellin-convolutions, which occurred in Eqs. (3.65, 3.66) and Eq. (4.46). These are convolutions with leading order splitting functions. We use the parameter  $\kappa = m^2/Q^2$  and refer to the alphabet in Eqs. (3.40-3.51) for the iterated integrals. We use the short hand  $H_{\bar{a}} \equiv H_{\bar{a}}(\beta)$ .

$$\begin{aligned}
 P_{gq}^{(0)} \otimes h_{L,g}^{(1)} &= C_F T_F \left\{ 64\beta(1-z) \frac{1+6\kappa - (8\kappa+2)z - (8\kappa+2)z^2}{3z(1+4\kappa)} - \frac{64}{3} z(3+4\kappa z) \ln \left( \frac{1-\beta}{1+\beta} \right) \right. \\
 &\quad \left. + \frac{64}{3} \frac{4\kappa(1+3\kappa) - 6\kappa(1+4\kappa)z + 3(1+4\kappa)^2 z^2}{z(1+4\kappa)^{3/2}} \ln \left( \frac{\sqrt{1+4\kappa} - \beta}{\sqrt{1+4\kappa} + \beta} \right) \right\}, \tag{D.47}
 \end{aligned}$$

$$\begin{aligned}
 P_{gq}^{(0)} \otimes \bar{b}_{L,g}^{(1)} &= C_F T_F \left\{ -\frac{32(1-z)(3-4z-6z^2)\beta}{3z} + \frac{8}{3} z(3+4z\kappa) \ln^2 \left( \frac{1-\beta}{1+\beta} \right) \right. \\
 &\quad - \frac{64}{3} z(3+4z\kappa) \left[ \text{Li}_2 \left( \frac{1-\beta}{2} \right) - \text{Li}_2(1-\beta) - \text{Li}_2(-\beta) \right] \\
 &\quad - \frac{8}{3z(1+4\kappa)^{5/2}} \left[ 2\kappa^2(1+\kappa) - 3z\kappa^2(1+4\kappa) + 3z^2(1+4\kappa)^2(\kappa + \sqrt{1+4\kappa}) \right. \\
 &\quad \left. + 4z^3\kappa(1+4\kappa)^{5/2} \right] \ln^2(1-z) - \frac{8\kappa R_{66}}{3z(1+4\kappa)^{5/2}} \left[ \ln^2 \left( \frac{\sqrt{1+4\kappa} - 1}{\sqrt{1+4\kappa} + 1} \right) \right. \\
 &\quad \left. + \ln^2 \left( \frac{\sqrt{1+4\kappa} - \beta}{\sqrt{1+4\kappa} + \beta} \right) - 4 \ln(\kappa) \ln \left( \frac{\sqrt{1+4\kappa} - 1}{\sqrt{1+4\kappa} + 1} \right) - 8 \text{Li}_2 \left( \frac{1}{1 - \sqrt{1+4\kappa}} \right) \right. \\
 &\quad \left. + 8 \text{Li}_2 \left( \frac{1}{1 + \sqrt{1+4\kappa}} \right) + 8 \text{Li}_2 \left( \frac{\sqrt{1+4\kappa} - 1}{\sqrt{1+4\kappa} + 1} \right) - 8 \ln(2) \ln \left( \frac{\sqrt{1+4\kappa} - 1}{\sqrt{1+4\kappa} + 1} \right) \right\}
 \end{aligned}$$

$$\begin{aligned}
 & +8\text{Li}_2\left(\frac{\beta - \sqrt{1+4\kappa}}{\beta + \sqrt{1+4\kappa}}\right) - 8\text{Li}_2\left(\frac{(\sqrt{1+4\kappa}-1)(\sqrt{1+4\kappa}-\beta)}{(1+\sqrt{1+4\kappa})(\beta+\sqrt{1+4\kappa})}\right) \\
 & -2\ln(1-z)\ln\left(\frac{\sqrt{1+4\kappa}-1}{\sqrt{1+4\kappa}+1}\right) + \frac{64}{3}z(3+4z\kappa)\ln(\beta)\ln(2) \\
 & + \frac{16R_{70}}{3z(1+4\kappa)^{5/2}}\ln\left(\frac{\sqrt{1+4\kappa}-1}{\sqrt{1+4\kappa}+1}\right)\ln\left(\frac{\sqrt{1+4\kappa}-\beta}{\sqrt{1+4\kappa}+\beta}\right) \\
 & + \frac{32R_{68}}{3z(1+4\kappa)^{5/2}}\left[\text{Li}_2\left(\frac{\sqrt{1+4\kappa}-\beta}{\sqrt{1+4\kappa}+1}\right) + \text{Li}_2\left(\frac{\sqrt{1+4\kappa}-1}{\sqrt{1+4\kappa}+\beta}\right)\right] \\
 & - \frac{32R_{67}}{3z(1+4\kappa)^{3/2}}\ln\left(\frac{\sqrt{1+4\kappa}-\beta}{\sqrt{1+4\kappa}+\beta}\right) - \frac{32R_{65}}{3z(1+4\kappa)^{3/2}}\left[2\text{Li}_2\left(-\frac{\beta}{\sqrt{1+4\kappa}}\right)\right. \\
 & \left.- 2\text{Li}_2\left(\frac{\beta}{\sqrt{1+4\kappa}}\right) + \text{Li}_2\left(\frac{\sqrt{1+4\kappa}-1}{\sqrt{1+4\kappa}-\beta}\right) + \text{Li}_2\left(\frac{\sqrt{1+4\kappa}+\beta}{\sqrt{1+4\kappa}+1}\right)\right. \\
 & \left.- 2\ln(\beta)\ln\left(\frac{\sqrt{1+4\kappa}-\beta}{\sqrt{1+4\kappa}+\beta}\right)\right] + \frac{32}{3z(1+4\kappa)^{5/2}}\left[6\kappa^2(1+\kappa) - 9z\kappa^2(1+4\kappa)\right. \\
 & \left.+ 3z^2(1+4\kappa)^2(3\kappa - \sqrt{1+4\kappa}) - 4z^3\kappa(1+4\kappa)^{5/2}\right]\zeta_2 + \frac{32\beta R_{64}}{3z(1+4\kappa)}\ln(1-z) \\
 & + \frac{16R_{69}}{3z(1+4\kappa)^{5/2}}\ln(1-z)\ln\left(\frac{\sqrt{1+4\kappa}-\beta}{\sqrt{1+4\kappa}+\beta}\right) - \frac{16}{3}z(3+4z\kappa)\left[\ln\left(\frac{1-\beta}{1+\beta}\right)\right. \\
 & \left.- \ln(z) + 2\ln(\beta) - \ln(\kappa)\right]\ln(1-z) - \frac{32\beta R_{64}}{3z(1+4\kappa)}\ln(z) \\
 & + \frac{16}{3}z(3+4z\kappa)\left[\ln\left(\frac{1-\beta}{1+\beta}\right) + 2\ln(\beta) - \ln(\kappa)\right]\ln(z) - \frac{8}{3}z(3+4z\kappa)\ln^2(z) \\
 & + \frac{64\beta R_{64}}{3z(1+4\kappa)}\ln(\beta) - \frac{32}{3}z(3+4z\kappa)\left[\ln\left(\frac{1-\beta}{1+\beta}\right) - \ln(\kappa)\right]\ln(\beta) \\
 & - \left[\frac{32}{3}\left(3 - 6z - 4z^2\kappa - \frac{1+6\kappa}{z(1+4\kappa)}\right) + \frac{16}{3}z(3+4z\kappa)\ln(\kappa)\right]\ln\left(\frac{1-\beta}{1+\beta}\right) \\
 & \left. - \frac{8}{3}z(3+4z\kappa)\ln^2(\kappa)\right\}, \tag{D.48}
 \end{aligned}$$

where we introduced the polynomials

$$R_{64} = 6\kappa + (8\kappa + 2)z^3 - (14\kappa + 3)z + 1, \tag{D.49}$$

$$R_{65} = 4\kappa(1 + 3\kappa) + 3(1 + 4\kappa)^2z^2 - 6\kappa(1 + 4\kappa)z, \tag{D.50}$$

$$R_{66} = 2\kappa(1 + \kappa) + 3(1 + 4\kappa)^2z^2 - 3\kappa(1 + 4\kappa)z, \tag{D.51}$$

$$R_{67} = 24\kappa^2 + 12\kappa - 3(1 + 4\kappa)^2z + 6(1 + 4\kappa)^2z^2 + 1, \tag{D.52}$$

$$R_{68} = 4\kappa(11\kappa^2 + 6\kappa + 1) - 6\kappa(12\kappa^2 + 7\kappa + 1)z + 3(1 + 2\kappa)(1 + 4\kappa)^2z^2, \tag{D.53}$$

$$R_{69} = 2\kappa(23\kappa^2 + 13\kappa + 2) - 3\kappa(28\kappa^2 + 15\kappa + 2)z + 3(1 + 3\kappa)(1 + 4\kappa)^2z^2, \tag{D.54}$$

$$R_{70} = 2\kappa(25\kappa^2 + 15\kappa + 2) - 3\kappa(36\kappa^2 + 17\kappa + 2)z + 3(1 + 5\kappa)(1 + 4\kappa)^2z^2. \tag{D.55}$$

For  $F_1$  the corresponding quantities read

$$\begin{aligned}
 P_{gq}^{(0)} \otimes h_{1,g}^{(1)} & = C_{FTF} \left\{ (1+z-2z\kappa) \left[ -32\ln^2\left(\frac{1-\beta}{1+\beta}\right) - 64\text{Li}_2\left(\frac{1-\beta}{2}\right) + 64\text{Li}_2\left(\frac{1+\beta}{2}\right) \right] \right. \\
 & \left. - 64\text{Li}_2\left(\frac{\beta+1}{1-\sqrt{1+4\kappa}}\right) + 64\text{Li}_2\left(\frac{\beta-1}{\sqrt{1+4\kappa}-1}\right) + 64\text{Li}_2\left(\frac{1-\beta}{1+\sqrt{1+4\kappa}}\right) \right\}
 \end{aligned}$$

$$\begin{aligned}
 & -64\text{Li}_2\left(\frac{1+\beta}{1+\sqrt{1+4\kappa}}\right) + \left(-64\ln(1+\beta) - 128\ln(1+\sqrt{1+4\kappa})\right. \\
 & + 128\ln(\beta+\sqrt{1+4\kappa}) - 64\ln\left(\frac{\sqrt{1+4\kappa}-1}{\sqrt{1+4\kappa}+1}\right) + 64\ln\left(\frac{\sqrt{1+4\kappa}-\beta}{\sqrt{1+4\kappa}+\beta}\right) \\
 & \left.+ 64\ln(2)\right)\ln\left(\frac{1-\beta}{1+\beta}\right) - \frac{64(1-z)\beta}{3z(1+4\kappa)}(3z(1+4\kappa) + 2z^2(1-2\kappa)(1+4\kappa) \\
 & + 2(1+7\kappa)) - \frac{32}{3}(3-3z-4z^2(1-2\kappa)(1+2\kappa))\ln\left(\frac{1-\beta}{1+\beta}\right) \\
 & \left. - \frac{128}{3z(1+4\kappa)^{3/2}}(1+9(1-z)\kappa + 2(7-18z)\kappa^2)\ln\left(\frac{\sqrt{1+4\kappa}-\beta}{\sqrt{1+4\kappa}+\beta}\right)\right\}, \quad (\text{D.56})
 \end{aligned}$$

$$\begin{aligned}
 P_{gq}^{(0)} \otimes \bar{b}_{1,g}^{(1)} &= C_F T_F \left\{ \frac{2(1+k)^3 R_{71}}{3k^4 z} \left[ k\text{H}_{w_1} - k\text{H}_{w_2} + \ln(1-k^2) - \ln(1-z) \right] \text{H}_0 + \frac{32R_{72}}{3z} (\text{H}_{w_1} \right. \\
 & + \text{H}_{w_2}) - \frac{R_{73}}{6k^2 z} \ln(1-k)\text{H}_{w_2} + \frac{R_{74}}{6k^2 z} [\ln(1-k)\text{H}_{w_1} + \ln(1+k)\text{H}_{w_2}] + \frac{8R_{75}}{3z} \\
 & \times \left[ \text{H}_{w_1,-1} - \text{H}_{w_2,1} + \text{H}_{w_2,-1} + 2\ln(k)(\text{H}_{w_1} + \text{H}_{w_2}) \right] + \frac{96kz(1+z)}{3z} (\text{H}_{w_1,-1} - \text{H}_{w_2,1} \\
 & - \text{H}_{w_2,-1}) + \frac{-16R_{75}}{3z} \left( \text{H}_{w_1,0} + \text{H}_{w_2,0} + \frac{1}{2}\text{H}_{w_1,1} \right) + \frac{96kz(1+z)}{3z} \text{H}_{w_1,1} \\
 & - \frac{(1-3k^2)R_{76}}{6k^3 z} \left[ \ln^2(1-k) - \ln^2(1+k) - \ln(1-z)\{\ln(1-k) - \ln(1+k)\} \right] \\
 & + \frac{R_{77}}{6k^2 z} \ln(1+k)\text{H}_{w_1} + \frac{16R_{78}}{3k^4} \text{H}_1 \text{H}_{-1} + \frac{16R_{79}}{3k^4} \left[ 2\text{H}_{0,1} - 2\text{H}_{-1,0} - 2\text{H}_1 \text{H}_0 \right. \\
 & \left. - [\ln(1-k^2) - 2\ln(k)](\text{H}_1 + \text{H}_{-1}) \right] + \frac{16(1-z)\beta R_{80}}{3k^2 z} - \frac{8R_{81}}{3k^4 z} \ln(2) \left[ \ln(1-z) \right. \\
 & \left. - \ln(1-k^2) - k(\text{H}_{w_1} - \text{H}_{w_2}) \right] + \frac{16R_{82}}{3k^4 z(1-\beta)} (z - k^2(1 - (1-z)\beta)) \left[ \ln(1-k^2) \right. \\
 & \left. - 2\ln(k) \right] - \frac{32(1-z)\beta R_{83}}{3k^2 z} \text{H}_0 - \frac{8R_{84}}{3k^4 z} \text{H}_1 + \frac{8R_{85}}{3k^4 z} \text{H}_{-1} - \frac{8}{3} \left[ 3 + 9z \right. \\
 & \left. - \frac{(1+k^2)(1-3k^2)z^2}{k^4} \right] (\text{H}_1^2 - \text{H}_{-1}^2) + \frac{32}{3} \left[ 9 + 3z + \frac{(1+k^2)(1-3k^2)z^2}{k^4} \right] \text{H}_{-1,1} \\
 & + \left( \frac{16z}{k} - 16k(2+3z) \right) \left[ -2\text{H}_{w_1,1,0} - \text{H}_{w_1,1,1} + \text{H}_{w_1,1,-1} - 2\text{H}_{w_1,-1,0} - \text{H}_{w_1,-1,1} \right. \\
 & + \text{H}_{w_1,-1,-1} + 2\text{H}_{w_2,1,0} + \text{H}_{w_2,1,1} - \text{H}_{w_2,1,-1} + 2\text{H}_{w_2,-1,0} + \text{H}_{w_2,-1,1} \\
 & \left. - \text{H}_{w_2,-1,-1} - (\zeta_2 - \ln^2(2))(\text{H}_{w_1} - \text{H}_{w_2}) - (\text{H}_{w_1,1} + \text{H}_{w_1,-1} - \text{H}_{w_2,1} - \text{H}_{w_2,-1}) \right. \\
 & \left. \times \{\ln(1-k^2) - 2\ln(k)\} \right] + (2 + (3 - \frac{1}{k^2})z) \left[ -\frac{8}{3}(\text{H}_{-1}^3 + \text{H}_1^3) - 32\text{H}_{-1,1}\text{H}_{-1} \right. \\
 & + 32\text{H}_{-1,0,1} + 64\text{H}_{-1,1,0} + 64\text{H}_{-1,1,1} + 32\text{H}_{-1,-1,0} + 64\text{H}_{-1,-1,1} - 32\text{H}_{0,1,1} \\
 & + 16[\ln(1-z) - \ln(1-k^2)](\ln^2(2) - \zeta_2) + 8(\text{H}_{-1} - 2\text{H}_0)\text{H}_1^2 + 8(\text{H}_{-1}^2 \\
 & + 4\text{H}_{0,1} - 4\text{H}_{-1,0} - 4\text{H}_{-1,1})\text{H}_1 - 8[\ln(1-k^2) - 2\ln(k)]\{2\text{H}_{-1}\text{H}_1 - 4\text{H}_{-1,1} \\
 & \left. + \text{H}_1^2 - \text{H}_{-1}^2\} \right] \left. \right\}, \quad (\text{D.57})
 \end{aligned}$$

with the polynomials

$$R_{71} = 99k^6 - 297k^5 + 270k^4 - 18k^3 - 77k^2 + 39k - 8, \quad (\text{D.58})$$

$$R_{72} = k^4 + k^2(3z + 2) + 6z - 3, \quad (\text{D.59})$$

$$R_{73} = 9k^8 + 48k^6(3z - 2) + k^4(214 - 552z) + 48k^2(9z - 5) - 24z + 17, \quad (\text{D.60})$$

$$R_{74} = 9k^8 + 48k^6(3z - 4) + 6k^4(4z + 57) - 16k^2(9z + 1) - 24z + 17, \quad (\text{D.61})$$

$$R_{75} = 3k^4 - 2k^2(9z + 2) + 18z - 7, \quad (\text{D.62})$$

$$R_{76} = 3k^6 + k^4(48z - 47) + k^2(77 - 72z) + 24z - 17, \quad (\text{D.63})$$

$$R_{77} = -9k^8 - 48k^6(3z - 2) + k^4(552z - 214) - 48k^2(9z - 5) + 24z - 17, \quad (\text{D.64})$$

$$R_{78} = 3k^4(z^2 - z - 3) + 2k^2z^2 - z^2, \quad (\text{D.65})$$

$$R_{79} = 3k^4(z^2 + z - 1) + 2k^2z^2 - z^2, \quad (\text{D.66})$$

$$R_{80} = 2k^4 + k^2(2z^2 + 9z + 12) - 2z^2, \quad (\text{D.67})$$

$$R_{81} = 9k^4z(z + 3) + 2k^2(3z^2 - 9z + 5) - 3z^2 + 3z - 2, \quad (\text{D.68})$$

$$R_{82} = 3k^4 - k^2(6z^2 + 6z + 7) + 2z^2, \quad (\text{D.69})$$

$$R_{83} = -3k^4 + k^2(6z^2 + 6z + 7) - 2z^2, \quad (\text{D.70})$$

$$R_{84} = 6k^6(\beta(z - 1) + 1) + k^4(14(\beta - 1) - 2(6\beta - 5)z^3 + 3z^2 - 2(\beta - 15)z) \\ + k^2z^2(-4\beta + 4(\beta - 1)z + 3) + 2z^3, \quad (\text{D.71})$$

$$R_{85} = 6k^6(\beta(z - 1) - 1) - k^4(-14(\beta + 1) + 2(6\beta + 5)z^3 + 3z^2 + 2(\beta + 15)z) \\ + k^2z^2(-4\beta + 4(\beta + 1)z - 3) - 2z^3. \quad (\text{D.72})$$

For the polarized Wilson coefficient  $H_{g_1}^{(2),\text{PS}}$  we find

$$P_{gq}^{(0)} \otimes h_{g_1}^{(1)} = C_F T_F \left\{ -192(1 - z)\beta + 32(1 + 2z)\sqrt{1 + 4\kappa} \ln \left( \frac{\sqrt{1 + 4\kappa} - \beta}{\sqrt{1 + 4\kappa} + \beta} \right) \right. \\ + \left[ -64(1 + z) \ln(1 + \sqrt{1 + 4\kappa}) + 64(1 + z) \ln(\beta + \sqrt{1 + 4\kappa}) \right. \\ - 32(1 + z) \ln \left( \frac{\sqrt{1 + 4\kappa} - 1}{\sqrt{1 + 4\kappa} + 1} \right) + 32(1 + z) \ln \left( \frac{\sqrt{1 + 4\kappa} - \beta}{\sqrt{1 + 4\kappa} + \beta} \right) \\ \left. \left. - 16(7 - z(1 - 4\kappa)) + 32(1 + z) \ln(2) - 32(1 + z) \ln(1 + \beta) \right] \ln \left( \frac{1 - \beta}{1 + \beta} \right) \right. \\ - 32(1 + z) \text{Li}_2 \left( \frac{1 - \beta}{2} \right) + 32(1 + z) \text{Li}_2 \left( \frac{1 + \beta}{2} \right) - 16(1 + z) \ln^2 \left( \frac{1 - \beta}{1 + \beta} \right) \\ - 32(1 + z) \text{Li}_2 \left( \frac{1 + \beta}{1 - \sqrt{1 + 4\kappa}} \right) + 32(1 + z) \text{Li}_2 \left( \frac{\beta - 1}{\sqrt{1 + 4\kappa} - 1} \right) \\ \left. \left. + 32(1 + z) \text{Li}_2 \left( \frac{1 - \beta}{1 + \sqrt{1 + 4\kappa}} \right) - 32(1 + z) \text{Li}_2 \left( \frac{1 + \beta}{1 + \sqrt{1 + 4\kappa}} \right) \right\}, \quad (\text{D.73})$$

$$P_{gq}^{(0)} \otimes \bar{b}_{g_1}^{(1)} = C_F T_F \left\{ 208(1 - z)\beta + \frac{16(1 - k^2)}{k} \ln^2(1 - k) - \frac{4}{k^2} (2k^2z - 7k^2 - z) \right\} \\ \left\{ 4\text{H}_1\text{H}_0 + 2 \ln(1 - k) [\text{H}_1 + \text{H}_{-1}] - 4 \ln(k) [\text{H}_1 + \text{H}_{-1}] + 2 \ln(1 + k) [\text{H}_1 + \text{H}_{-1}] + \text{H}_1^2 \right. \\ \left. - 2\text{H}_1\text{H}_{-1} - \text{H}_{-1}^2 - 4\text{H}_{0,1} + 4\text{H}_{-1,0} + 4\text{H}_{-1,1} \right\} - \frac{8}{k^2} (4k^2 + z + 7k^2z - 12k^2\beta) \\ + 12k^2z\beta \text{H}_{-1} - \frac{8}{k^2} (4k^2 + z + 7k^2z + 12k^2\beta - 12k^2z\beta) \text{H}_1$$

$$\begin{aligned}
 & +32(1+2z) \left\{ (1+\ln(k)) [\mathbf{H}_{w_1} + \mathbf{H}_{w_2}] - \mathbf{H}_{w_1,0} - \mathbf{H}_{w_2,0} - \frac{1}{2} [\mathbf{H}_{w_1,1} - \mathbf{H}_{w_1,-1} \right. \\
 & \left. + \mathbf{H}_{w_2,1} - \mathbf{H}_{w_2,-1}] \right\} - 96(1-z)\beta [\ln(1-k^2) - 2\ln(k) + 2\mathbf{H}_0] \\
 & - 16 \left( (k^2+2z)\ln(1-k) + (2-k^2+2z)\ln(1+k) \right) \mathbf{H}_{w_1} \\
 & - 16 \left( (2-k^2+2z)\ln(1-k) + (k^2+2z)\ln(1+k) \right) \mathbf{H}_{w_2} \\
 & + 8(1+z) \left[ \mathbf{H}_1 \mathbf{H}_{-1}^2 - 4\mathbf{H}_{0,1,1} + 4\mathbf{H}_{-1,0,1} + 8\mathbf{H}_{-1,1,0} + 8\mathbf{H}_{-1,1,1} + 4\mathbf{H}_{-1,-1,0} \right. \\
 & \left. + 8\mathbf{H}_{-1,-1,1} - \frac{1}{3} [\mathbf{H}_1^3 + \mathbf{H}_{-1}^3] + [\mathbf{H}_1^2 - 4\mathbf{H}_{-1,1}] \mathbf{H}_{-1} + [4\mathbf{H}_{0,1} - 4\mathbf{H}_{-1,0} - 4\mathbf{H}_{-1,1} \right. \\
 & \left. - 2\mathbf{H}_1 \mathbf{H}_0] \mathbf{H}_1 + [\mathbf{H}_{-1}^2 - \mathbf{H}_1^2 - 2\mathbf{H}_1 \mathbf{H}_{-1} + 4\mathbf{H}_{-1,1}] (\ln(1-k^2) - 2\ln(k)) \right. \\
 & \left. + 2(\zeta_2 - \ln^2(2)) [\ln(1-k^2) - \ln(1-z)] \right] + 32 [\ln(1-k^2) - \ln(1-z)] \ln(2) \\
 & + 16k(1+z) \left[ 2\mathbf{H}_{w_1,1,0} + \mathbf{H}_{w_1,1,1} - \mathbf{H}_{w_1,1,-1} + 2\mathbf{H}_{w_1,-1,0} + \mathbf{H}_{w_1,-1,1} - \mathbf{H}_{w_1,-1,-1} \right. \\
 & \left. - 2\mathbf{H}_{w_2,1,0} - \mathbf{H}_{w_2,1,1} + \mathbf{H}_{w_2,1,-1} - 2\mathbf{H}_{w_2,-1,0} - \mathbf{H}_{w_2,-1,1} + \mathbf{H}_{w_2,-1,-1} \right. \\
 & \left. + (\ln(1-k^2) - 2\ln(k)) [\mathbf{H}_{w_1,1} + \mathbf{H}_{w_1,-1} - \mathbf{H}_{w_2,1} - \mathbf{H}_{w_2,-1}] \right. \\
 & \left. + (\zeta_2 - \ln^2(2)) [\mathbf{H}_{w_1} - \mathbf{H}_{w_2}] \right] + 32k \ln(2) [\mathbf{H}_{w_1} - \mathbf{H}_{w_2}] \\
 & \left. - \frac{16(1-k^2)}{k} \left( \ln^2(1+k) + \ln(1-z) [\ln(1-k) - \ln(1+k)] \right) \right\}. \tag{D.74}
 \end{aligned}$$

## D.5. Remarks on the encountered iterated integrals

In this calculation a large number of generalized iterated integrals appear. If no elliptic letter is present, it is possible to represent them using harmonic polylogarithms when the letters do not involve kinematic variables or polylogarithms at involved arguments. The expressions become large already in simple situations. In total about 1050 logarithms, di- and trilogarithms contribute. In a series of cases a further elliptic letter is integrated over these structures.

A few examples are given in the following. Let us refer to the letters  $f_{w_9}$  and  $f_{w_6}$ . The corresponding iterated integral reads

$$\begin{aligned}
 H_{w_9, w_6}(\beta) = & \frac{1 - \beta^2(1-z)}{2k(1-z)^2 z(z+1)} \left\{ -\text{Li}_2 \left[ \frac{\sqrt{z+1}(k+z)}{z\sqrt{z+1} + k \left( (1-z)\sqrt{z\beta^2+1} + \sqrt{z+1} \right)} \right] \right. \\
 & + \text{Li}_2 \left[ \frac{\sqrt{z+1}((z-1)\beta k + k + z)}{z\sqrt{z+1} + k \left( (1-z)\sqrt{z\beta^2+1} + \sqrt{z+1} \right)} \right] \\
 & - \text{Li}_2 \left[ \frac{\sqrt{z+1}(k+z)}{z\sqrt{z+1} - k \left( (1-z)\sqrt{z\beta^2+1} - \sqrt{z+1} \right)} \right] \\
 & \left. + \text{Li}_2 \left[ \frac{\sqrt{z+1}((z-1)\beta k + k + z)}{z\sqrt{z+1} - k \left( (1-z)\sqrt{z\beta^2+1} - \sqrt{z+1} \right)} \right] + \ln(k+z) \right\} - \ln(1-\beta^2)
 \end{aligned}$$

$$\begin{aligned}
 & -\ln\left(-\frac{k(z-1)\sqrt{\beta^2 z+1}}{k\left(-z\sqrt{\beta^2 z+1}+\sqrt{\beta^2 z+1}+\sqrt{z+1}\right)+\sqrt{z+1}z}\right) \\
 & -\ln\left(\frac{k(z-1)\sqrt{\beta^2 z+1}}{k\left(-\left(1-z\right)\sqrt{\beta^2 z+1}+\sqrt{z+1}\right)+z\sqrt{z+1}}\right)+\ln(\beta^2 z+1)\Big\} \\
 & +\ln(\beta k(z-1)+k+z) \\
 & \times\left\{\ln\left(\frac{k(z-1)\left(\sqrt{\beta^2 z+1}+\beta\sqrt{z+1}\right)}{k\left(\left(1-z\right)\sqrt{\beta^2 z+1}+\sqrt{z+1}\right)+z\sqrt{z+1}}\right)\right. \\
 & \left.+\ln\left(\frac{k(z-1)\left(\sqrt{\beta^2 z+1}-\beta\sqrt{z+1}\right)}{k\left(-\left(1-z\right)\sqrt{\beta^2 z+1}+\sqrt{z+1}\right)+z\sqrt{z+1}}\right)\right\}. \tag{D.75}
 \end{aligned}$$

Examples of the contributing functions are

$$\text{Li}_2\left(\frac{\sqrt{1+z}(k+z)}{z\sqrt{1+z}+k\left(\sqrt{1+z}-\sqrt{1+z\beta^2+z\sqrt{1+z\beta^2}}\right)}\right), \tag{D.76}$$

$$\text{Li}_2\left(\frac{k\sqrt{1-z^2}(-z+k(1+(1-z)\beta))}{-zk\sqrt{1-z^2}+k(k\sqrt{1-z^2}+\sqrt{k^2-z^2}(1-z))}\right), \tag{D.77}$$

$$\text{Li}_3\left(-\frac{2(1-k)z\beta}{(1-\beta)(z-k(1+(1-z)\beta))}\right) \tag{D.78}$$

and logarithms of similar arguments.

Finally, we expand one of the iterated integrals, containing an elliptic letter, in the ratio  $m^2/Q^2$ . While the asymptotic expansion of the functions in Appendix D.4 is straight forward after the integration into polylogarithmic expressions, the asymptotic expansion of the Kummer-elliptic integrals is more involved. Here we rely heavily on the techniques developed in the context of Ref. [4] for the expansion of massive iterative integrals in the Drell-Yan process. The main idea is to perform the first integration analytically and then regularize the integrand in the limit  $Q^2 \gg m^2$  before the expansion. Since we aim for a deeper expansion in this paper, the term for the regularization turns out to be a power series in  $\kappa$ . For example, we find

$$\begin{aligned}
 \text{H}_{w_{10},w_7}(\beta) &= \frac{1}{1-z}\left\{\frac{1}{4}\ln^2\left(\frac{m^2}{Q^2}\right)+\frac{1}{2}(\ln(1-z)-\ln(2)-2\ln(1-\sqrt{z}))\ln\left(\frac{m^2}{Q^2}\right)\right. \\
 & +\left(2\ln(1-z)-\frac{5}{4}\ln(z)\right)\ln(1-\sqrt{z})-\frac{3}{4}\ln^2(1-\sqrt{z})-\ln^2(1-z) \\
 & +\frac{1}{2}\ln(1-z)\ln(z)-\frac{1}{16}\ln^2(z)-\text{Li}_2(1-\sqrt{z})-\text{Li}_2(\sqrt{z})-\frac{1}{2}\text{Li}_2\left(\frac{2\sqrt{z}}{1+\sqrt{z}}\right) \\
 & -\text{Li}_2\left(\frac{1}{2}(1-\sqrt{z})\right)-\frac{1}{2}\text{Li}_2\left(-\frac{1-\sqrt{z}}{2\sqrt{z}}\right)+\frac{11}{4}\zeta_2+\frac{1}{4}\left(6\ln(1-z)\right. \\
 & \left.-6\ln(1-\sqrt{z})-\ln(z)\right)\ln(2)-\frac{1}{4}\ln^2(2)+\frac{m^2}{Q^2}\left[\frac{1}{2}\ln^2\left(\frac{m^2}{Q^2}\right)\right. \\
 & \left.-\left(\frac{5-10\sqrt{z}-3z}{4(1-z)}+2\ln(1-\sqrt{z})-\ln(1-z)+\ln(2)\right)\ln\left(\frac{m^2}{Q^2}\right)\right. \\
 & \left.+\frac{1-8\sqrt{z}+z}{4(1-z)}+\left(\frac{5+6\sqrt{z}-3z}{2(1-z)}+4\ln(1-z)-\frac{5}{2}\ln(z)\right)\ln(1-\sqrt{z})\right\}
 \end{aligned}$$



$$\begin{aligned}
 & -\frac{3}{2} \ln^2(1 - \sqrt{z}) - \left( \frac{5 + 22\sqrt{z} - 3z}{4(1-z)} - \ln(z) \right) \ln(1-z) - 2 \ln^2(1-z) \\
 & -\frac{1}{8} \ln^2(z) - 2\text{Li}_2(1 - \sqrt{z}) - 2\text{Li}_2(\sqrt{z}) - \text{Li}_2\left(\frac{2\sqrt{z}}{1 + \sqrt{z}}\right) \\
 & -2\text{Li}_2\left(\frac{1}{2}(1 - \sqrt{z})\right) - \text{Li}_2\left(-\frac{1 - \sqrt{z}}{2\sqrt{z}}\right) + \frac{2}{(1-z)} \sqrt{z} \ln(z) + \frac{11}{2} \zeta_2 \\
 & + \left( \frac{3 + 10\sqrt{z} - z}{2(1-z)} - 3 \ln(1 - \sqrt{z}) + 3 \ln(1-z) - \frac{1}{2} \ln(z) \right) \ln(2) - \frac{1}{2} \ln^2(2) \Big] \\
 & + \left( \frac{m^2}{Q^2} \right)^2 \left[ -\frac{1}{2} \ln^2\left(\frac{m^2}{Q^2}\right) + \left( -\frac{15(1+z^2) - 6z - 100\sqrt{z}(1+z)}{32(1-z)^2} + 2 \ln(1 - \sqrt{z}) \right. \right. \\
 & \left. \left. - \ln(1-z) + \ln(2) \right) \ln\left(\frac{m^2}{Q^2}\right) + \left( \frac{15 - 6z + 15z^2 + 28\sqrt{z} + 28z^{3/2}}{16(1-z)^2} - 4 \ln(1-z) \right. \right. \\
 & \left. \left. + \frac{5}{2} \ln(z) \right) \ln(1 - \sqrt{z}) + \frac{3}{2} \ln^2(1 - \sqrt{z}) + \left( -\frac{3(5 - 2z + 5z^2 + 52\sqrt{z} + 52z^{3/2})}{32(1-z)^2} \right. \right. \\
 & \left. \left. - \ln(z) \right) \ln(1-z) + 2 \ln^2(1-z) + \frac{1}{8} \ln^2(z) + 2\text{Li}_2(1 - \sqrt{z}) + \text{Li}_2\left(-\frac{1 - \sqrt{z}}{2\sqrt{z}}\right) \right. \\
 & \left. + 2\text{Li}_2(\sqrt{z}) + \text{Li}_2\left(\frac{2\sqrt{z}}{1 + \sqrt{z}}\right) + 2\text{Li}_2\left(\frac{1}{2}(1 - \sqrt{z})\right) + \frac{2(1+z)}{(1-z)^2} \sqrt{z} \ln(z) \right. \\
 & \left. + \frac{97 - 202z + 33z^2 - 324\sqrt{z} + 316z^{3/2}}{64(1-z)^2} + \left( \frac{7(1+z^2) + 10z + 60\sqrt{z}(1+z)}{16(1-z)^2} \right. \right. \\
 & \left. \left. + 3 \ln(1 - \sqrt{z}) - 3 \ln(1-z) + \frac{1}{2} \ln(z) \right) \ln(2) - \frac{11}{2} \zeta_2 + \frac{1}{2} \ln^2(2) \Big] \Big\} \\
 & + O(\kappa^3 \ln^2(\kappa)), \tag{D.79}
 \end{aligned}$$

and similar expressions for the other Kummer-elliptic integrals. When calculating the complete expansion all dependence on  $\sqrt{z}$  drops out of the Wilson coefficients. We did not exploit here the well-known relations for the dilogarithm of different arguments [265, 266].



# E. Initial State Radiation to $e^+ e^-$ Annihilation Revisited – Computational Details

## E.1. Phase Space Parametrization

### Fermion Pair Radiation

For massive fermion pair radiation we only encounter  $2 \rightarrow 3$  scattering with the kinematics

$$p_- + p_+ = q + k_- + k_+ \quad (\text{E.1})$$

with

$$\begin{aligned} (p_- + p_+)^2 &= s, \\ q^2 &= s', \\ p_-^2 = p_+^2 = k_-^2 = k_+^2 &= m^2. \end{aligned} \quad (\text{E.2})$$

We also introduce the invariants

$$(k_+ + q)^2 = s_3, \quad (\text{E.3})$$

$$(k_- + q)^2 = s_4, \quad (\text{E.4})$$

$$(k_- + k_2)^2 = s'', \quad (\text{E.5})$$

which satisfy the identity

$$s_3 + s_4 + s'' = s + s' + m^2. \quad (\text{E.6})$$

The phase space integral is given by

$$\begin{aligned} \int d\text{PS}_3 &= \frac{1}{(2\pi)^6} \int d^4q \int d^4k_- \int d^4k_+ \left\{ \delta(q^2 - s') \delta(k_-^2 - m^2) \right. \\ &\quad \left. \times \delta(k_+^2 - m^2) \delta^{(4)}(p_- + p_+ - q - k_- - k_+) \right\} \\ &= \frac{1}{(2\pi)^6} \int d^4k_1 \int d^4k_2 \left\{ \delta([p_- + p_+ - k_1 - k_2]^2 - s') \delta(k_1^2 - m^2) \right. \\ &\quad \left. \times \delta(k_2^2 - m^2) \right\} \\ &= \frac{1}{(2\pi)^5} \int dk_1^0 \int d|\vec{k}_1| \int d\cos(\chi) \int dk_2^0 \int d|\vec{k}_2| \int_{-1}^1 d\cos(\theta) \int_0^{2\pi} d\phi \\ &\quad \times \left\{ |\vec{k}_1|^2 |\vec{k}_2|^2 \frac{\delta(\cos(\chi) - \cos(\chi_0))}{2|\vec{k}_1||\vec{k}_2|} \frac{\delta(|\vec{k}_1| - \sqrt{(k_1^0)^2 - m^2})}{2|\vec{k}_1|} \frac{\delta(|\vec{k}_2| - \sqrt{(k_2^0)^2 - m^2})}{2|\vec{k}_2|} \right\} \\ &= \frac{1}{4(2\pi)^5} \int dk_1^0 \int dk_2^0 \int_{-1}^1 d\cos(\theta) \int_0^\pi d\phi \end{aligned}$$

$$\begin{aligned}
 &= \frac{1}{(4\pi)^4} \frac{1}{2\pi s} \int ds_3 \int ds_4 \int_{-1}^1 d \cos(\theta) \int_0^\pi d\phi \\
 &= \frac{1}{(4\pi)^4} \frac{1}{2\pi s} \int ds'' \int ds_3 \int_{-1}^1 d \cos(\theta) \int_0^\pi d\phi
 \end{aligned} \tag{E.7}$$

In deriving these relations the identities

$$\begin{aligned}
 \delta([p_- + p_+ - k_1 - k_2]^2 - s') &= \delta(s - s' - 2\sqrt{s}(k_1^0 + k_2^0) + 2m^2 + 2k_1 \cdot k_2) \\
 &= \delta(s - s' - 2\sqrt{s}(k_1^0 + k_2^0) + 2m^2 + 2k_1^0 k_2^0 - 2|\vec{k}_1||\vec{k}_2| \cos(\chi)) \\
 &= \frac{1}{2|\vec{k}_1||\vec{k}_2|} \delta(\cos(\chi) - \cos(\chi_0)),
 \end{aligned} \tag{E.8}$$

with

$$\cos(\chi_0) = \frac{s - s' + 2m^2 - 2\sqrt{s}(k_1^0 + k_2^0) + 2k_1^0 k_2^0}{2|\vec{k}_1||\vec{k}_2|}, \tag{E.9}$$

were used. The integration variables are transformed according to

$$\begin{aligned}
 s_3 &= (k_2 + q)^2 = (p_- + p_+ - k_1)^2 = s + m^2 - 2\sqrt{s}k_1^0, \\
 s_4 &= (k_1 + q)^2 = (p_- + p_+ - k_2)^2 = s + m^2 - 2\sqrt{s}k_2^0, \\
 ds_3 &= -2\sqrt{s}dk_1^0, \\
 ds_4 &= -2\sqrt{s}dk_2^0,
 \end{aligned} \tag{E.10}$$

and the symmetry of the angular integration allows to transform

$$\int_{-1}^1 d \cos(\theta) \int_0^{2\pi} d\phi = 2 \int_{-1}^1 d \cos(\theta) \int_0^\pi d\phi. \tag{E.11}$$

The phase space boundaries are given by

$$4m^2 < s'' < (\sqrt{s} - \sqrt{s'})^2, \tag{E.12}$$

$$s_3^- < s_3 < s_3^+, \tag{E.13}$$

where the explicit expressions for  $s_3^-$  and  $s_3^+$  are given by

$$s_3^\pm = \frac{1}{2} \left( s + s' - s'' + 2m^2 \pm \sqrt{1 - \frac{4m^2}{s''}} \lambda^{1/2}(s, s', s'') \right). \tag{E.14}$$

We can also change the order of integration in which case we obtain

$$(\sqrt{s} - m)^2 < s_3 < (\sqrt{s'} - m)^2, \tag{E.15}$$

$$s''^- < s'' < s''^+ \tag{E.16}$$

whit the explicit expressions

$$s''^\pm = \frac{1}{2s_3} \left( (s - s_3)(s_3 - s') + m^2(s + 2s_3 + s') - m^4 \pm \lambda^{1/2}(s, s_3, m^2) \lambda^{1/2}(s', s_3, m^2) \right). \tag{E.17}$$

We can use the following parametrization of the vectors:

$$\begin{aligned}
 p_- &= \frac{\sqrt{s}}{2} (1, 0, 0, \beta) \\
 p_+ &= \frac{\sqrt{s}}{2} (1, 0, 0, -\beta) \\
 k_1 &= \left( k_1^0, 0, |\vec{k}_1|s(\theta), |\vec{k}_1|c(\theta) \right) \tag{E.18}
 \end{aligned}$$

$$\begin{aligned}
 k_2 &= \left( k_2^0, |\vec{k}_2|s(\phi)s(\chi_0), |\vec{k}_2|(c(\chi_0)s(\theta) - c(\theta)c(\phi)s(\chi_0)), |\vec{k}_2|(c(\theta)c(\chi_0) + c(\phi)s(\theta)s(\chi_0)) \right) \\
 q &= p_- + p_+ - k_1 - k_2 \tag{E.19}
 \end{aligned}$$

with the abbreviation  $c(x) = \cos(x)$  and  $s(x) = \sin(x)$ . The missing components of the vectors are given by

$$\begin{aligned}
 k_1^0 &= \frac{s - s_3 + m^2}{2\sqrt{s}}, & |\vec{k}_1| &= \frac{\lambda^{1/2}(s, s_3, m^2)}{2\sqrt{s}} \\
 k_2^0 &= \frac{s - s_4 + m^2}{2\sqrt{s}}, & |\vec{k}_2| &= \frac{\lambda^{1/2}(s, s_4, m^2)}{2\sqrt{s}} \tag{E.20}
 \end{aligned}$$

The direction of the 3-vector component of  $k_2$  is achieved by rotating  $\vec{k}_1$  with angle  $\chi_0$  around the  $x$ -axis and then with angle  $\phi_0$  around  $k_1$ . It is convenient to transform to the dimensionless variables

$$t = \frac{s'}{s}, \quad x = \frac{s_3}{s}, \quad y = \frac{4m^2}{s''}, \tag{E.21}$$

in the explicit calculations. Since all involved particles are massive the phase space integrals are convergent and do not need any kind of regularization.

### Photon Radiation

The  $2 \rightarrow 3$  scattering can be very similarly parametrized as before. However the replacements  $k_- \rightarrow k_1$  and  $k_+ \rightarrow k_2$  with

$$k_1^2 = k_2^2 = 0 \tag{E.22}$$

have to be made. Therefore the limit  $m \rightarrow 0$  has to be taken in the expressions given in the previous section. We will give the explicit expressions for completeness.

The phase space integral reads

$$\begin{aligned}
 \int d\text{PS}_3 &= \frac{1}{(2\pi)^6} \int d^4q \int d^4k_- \int d^4k_+ \left\{ \delta(q^2 - s') \delta(k_-^2 - m^2) \right. \\
 &\quad \left. \times \delta(k_+^2 - m^2) \delta^{(4)}(p_- + p_+ - q - k_- - k_+) \right\} \\
 &= \frac{1}{(4\pi)^4} \frac{1}{2\pi s} \int ds_3 \int ds_4 \int_{-1}^1 d\cos(\theta) \int_0^\pi d\phi \tag{E.23}
 \end{aligned}$$

with the explicit parametrization of the vectors

$$\begin{aligned}
 p_- &= \frac{\sqrt{s}}{2} (1, 0, 0, \beta) \\
 p_+ &= \frac{\sqrt{s}}{2} (1, 0, 0, -\beta)
 \end{aligned}$$

$$k_1 = \frac{s - s_3}{2\sqrt{s}} (1, 0, s(\theta), c(\theta)) \quad (\text{E.24})$$

$$\begin{aligned} k_2 &= \frac{s - s_4}{2\sqrt{s}} (1, s(\phi)s(\chi_0), (c(\chi_0)s(\theta) - c(\theta)c(\phi)s(\chi_0)), (c(\theta)c(\chi_0) + c(\phi)s(\theta)s(\chi_0))) \\ q &= p_- + p_+ - k_1 - k_2. \end{aligned} \quad (\text{E.25})$$

The angle between the two photons is given by

$$\cos(\chi_0) = 1 - \frac{2ss''}{(s - s_3)(s - s_4)}. \quad (\text{E.26})$$

The phase space boundaries simplify to

$$\begin{aligned} \frac{ss'}{s_3} &\leq s_4 \leq s + s' - s_3, \\ s' &\leq s_3 \leq s. \end{aligned} \quad (\text{E.27})$$

They are symmetric in  $s_3$  and  $s_4$ .

It is also possible to only radiate one additional photon. In this case the phase space for  $2 \rightarrow 2$  scattering is needed. Using the kinematics

$$p_- + p_- = q + k \quad (\text{E.28})$$

with  $k^2 = 0$  it is given by

$$\begin{aligned} \int d\text{PS}_2 &= \int d^4q \int d^4k \delta(s - s') \delta(k^2) \delta^{(4)}(p_- + p_+ - q - k) \\ &= \frac{1}{(4\pi)^2} \frac{2}{s - s'} \int_{-1}^1 d\cos(\theta). \end{aligned} \quad (\text{E.29})$$

In this case the vectors can be parametrized by

$$\begin{aligned} p_- &= \frac{\sqrt{s}}{2} (1, 0, 0, \beta), \\ p_+ &= \frac{\sqrt{s}}{2} (1, 0, 0, -\beta), \\ k &= \frac{s - s'}{2\sqrt{s}} (1, 0, \sin(\theta), \cos(\theta)), \\ q &= p_- + p_+ - k. \end{aligned} \quad (\text{E.30})$$

## E.2. Angular Integrals

For the photon emission graphs we find the following denominators

$$\begin{aligned} D_1 &= (p_- - k_2)^2 - m^2, & D_2 &= (p_- - k_1)^2 - m^2, \\ D_3 &= (q - p_+)^2 - m^2, & D_4 &= (q - p_-)^2 - m^2, \\ D_5 &= (p_+ - k_2)^2 - m^2, & D_6 &= (p_+ - k_1)^2 - m^2. \end{aligned} \quad (\text{E.31})$$

For the angular integrals we again want to map to the angular integrals of the form

$$I_{l,k}^{d=4} = \int_0^\pi d\theta \int_0^\pi d\phi \frac{\sin(\theta)}{[a + b \cos(\theta)]^l} \frac{1}{[A + B \cos(\theta) + C \sin(\theta) \cos(\phi)]^k} \quad (\text{E.32})$$

For some denominator structures we have to use partial fractioning. Some cases are trivial, like

$$\frac{1}{D_2 D_6} = \frac{1}{s_3 - s} \left( \frac{1}{D_1} + \frac{1}{D_5} \right), \quad (\text{E.33})$$

$$\frac{1}{D_3 D_4} = \frac{1}{s'' - s} \left( \frac{1}{D_3} + \frac{1}{D_4} \right), \quad (\text{E.34})$$

$$\frac{1}{D_1 D_5} = \frac{1}{s_4 - s} \left( \frac{1}{D_5} + \frac{1}{D_6} \right). \quad (\text{E.35})$$

The more involved ones read

$$\frac{1}{D_1 D_2 D_3} = \frac{1}{s''} \left( \frac{1}{D_1 D_2} - \frac{1}{D_1 D_3} - \frac{1}{D_2 D_3} \right), \quad (\text{E.36})$$

$$\frac{1}{D_2 D_3 D_5} = \frac{1}{s' - s_3} \left( \frac{1}{D_2 D_3} + \frac{1}{D_2 D_5} - \frac{1}{D_3 D_5} \right), \quad (\text{E.37})$$

$$\frac{1}{D_1 D_3 D_6} = \frac{1}{s' - s_4} \left( \frac{1}{D_1 D_6} + \frac{1}{D_1 D_3} - \frac{1}{D_3 D_6} \right), \quad (\text{E.38})$$

$$\frac{1}{D_1 D_4 D_6} = -\frac{1}{s' - s_3} \left( \frac{1}{D_1 D_6} - \frac{1}{D_1 D_4} + \frac{1}{D_4 D_6} \right), \quad (\text{E.39})$$

$$\frac{1}{D_2 D_4 D_5} = \frac{1}{s' - s_4} \left( \frac{1}{D_2 D_5} + \frac{1}{D_4 D_5} - \frac{1}{D_2 D_4} \right) \quad (\text{E.40})$$

$$\frac{1}{D_4 D_5 D_6} = \frac{1}{s''} \left( \frac{1}{D_5 D_6} - \frac{1}{D_4 D_5} - \frac{1}{D_4 D_6} \right). \quad (\text{E.41})$$

For some combinations of denominators we have to interchange the parametrizations of  $k_-$  and  $k_+$  in order to arrive at angular integrals of the form (E.32).

If either  $l$  or  $k$  are negative we can use the relations given in Eqs. (D.38,D.39) for  $d = 4$  to arrive at the angular integrals. If both indices are negative we were not able to find a closed form in  $d$  dimensions. For  $d = 4$  we find

$$\begin{aligned} I_{-2,-2}^{d=4} = & 2\pi \frac{b^4 A^4 - 2ab^3 A^3 B - 2abAB(a^2 - 2b^2)(B^2 + C^2) - b^2 A^2(2b^2 B^2 - a^2(2B^2 - C^2))}{(a^2 - b^2)(A^2 - B^2 - C^2)X^2} \\ & - \frac{(B^2 + C^2)(2a^2 b^2 B^2 + b^4 C^2 - a^4(B^2 + C^2))}{(a^2 - b^2)(A^2 - B^2 - C^2)X^2} \\ & - b\pi \frac{2b^2 A^2 B + b^2 BC^2 + 2a^2 B(B^2 + C^2) - abA(4B^2 + 3C^2)}{X^{5/2}} \ln \left( \frac{aA - bB + \sqrt{X}}{aA - bB - \sqrt{X}} \right), \quad (\text{E.42}) \end{aligned}$$

$$I_{-2,-1}^{d=4} = \frac{2b(bA - aB)\pi}{(a^2 - b^2)X} + \pi \frac{a(B^2 + C^2) - bAB}{X^{3/2}} \ln \left( \frac{aA - bB + \sqrt{X}}{aA - bB - \sqrt{X}} \right), \quad (\text{E.43})$$

$$I_{-1,-2}^{d=4} = \frac{2\pi(a(B^2 + C^2) - bAB)}{(A^2 - B^2 - C^2)X} + \frac{b(bA - aB)\pi}{X^{3/2}} \ln \left( \frac{aA - bB + \sqrt{X}}{aA - bB - \sqrt{X}} \right), \quad (\text{E.44})$$

$$I_{-1,-1}^{d=4} = \frac{\pi}{\sqrt{X}} \ln \left( \frac{aA - bB + \sqrt{X}}{aA - bB - \sqrt{X}} \right), \quad (\text{E.45})$$

with  $X = (aA - bB)^2 - (a^2 - b^2)(A^2 - B^2 - C^2)$ . Note that we agree with the results given in [444, 446].





## F. Simplifying Polylogarithms at Complicated Arguments

During the calculation of phase space integrals using `Mathematica` a large amount of polylogarithms at complicated square root valued and imaginary arguments of one variable appeared although especially in the massless case the results were known to reduce to at most Nielsen integrals at simple arguments. A possibility of dealing with this problem is to find suitable integral transformations to avoid the integration into these complicated structures. Given the sheer amount of integrals and the not obvious transformations one has to use to arrive at simpler results this approach is hardly feasible for the projects presented in this thesis. In the following an algorithmic way is presented to map these expressions to generalized iterated integrals. Then build in functions of `HarmonicSums` can be used to reduce these integrals to an integral basis and in this way simplify these expressions to their final form.

The algorithm consists out of four steps:

1. Derive a first order differential equation with rational functions or iterated integrals with rational prefactors as inhomogeneity.
2. Integrate the differential equations in terms of iterated integrals.
3. Simplify the letters of the found iterated integrals.
4. Determine the integration constant by matching at  $x = 0$ .

The algorithm has similarities in construction and goals with the symbol calculus presented in [447]. However the approach presented here can also deal with square roots and retains all information of the integration constants.

Let's consider the illustrative example

$$f_a(x) = \ln(\sqrt{x} + i\sqrt{1-x}). \quad (\text{F.1})$$

1. We can derive the first order differential equation

$$\frac{d}{dx} f_a(x) = -\frac{i}{2\sqrt{x}\sqrt{1-x}} \quad (\text{F.2})$$

which already fulfills our requirements.

2. Integration leads to

$$F_a(x) = \int dx \frac{d}{dx} f_a(x) = -\frac{i}{2} G\left(\left\{\frac{1}{\sqrt{\tau}\sqrt{1-\tau}}\right\}, x\right) + C, \quad (\text{F.3})$$

which cannot be simplified by any means.

4. The iterated integral vanishes at  $x = 0$ . Therefore we find

$$C = f(0) = i\frac{\pi}{2} \quad (\text{F.4})$$

The representation in terms of iterated integrals therefore reads

$$f_a(x) = \ln(\sqrt{x} + i\sqrt{1-x}) = -\frac{i}{2}G\left(\left\{\frac{1}{\sqrt{\tau}\sqrt{1-\tau}}\right\}, x\right) + i\frac{\pi}{2}. \quad (\text{F.5})$$

For logarithms the above algorithm is hardly needed, since basically all relations can be found rather straight forwardly by elementary algebraic transformations. The real benefit of this approach shows for polylogarithms of higher weight. As an illustration we consider the function

$$f_b(x) = \text{Li}_2(1 - \sqrt{x} - i\sqrt{1-x}). \quad (\text{F.6})$$

1. Deriving with respect to  $x$  one finds

$$\frac{d}{dx}f_b(x) = \frac{1}{4}\left[\frac{1}{\sqrt{x}(1-\sqrt{x})} + \frac{i}{\sqrt{x}\sqrt{1-x}}\right]\ln(\sqrt{x} + i\sqrt{1-x}). \quad (\text{F.7})$$

Inserting the result for  $f_a(x)$  we arrive at a first order differential equation which fulfills the requirements. It is also beneficial to break the term into real and imaginary parts. Doing this one arrives at the final differential equation

$$\frac{d}{dx}f_b(x) = \frac{1}{8}\left[\frac{1}{\sqrt{x}\sqrt{1-x}} - \frac{i}{\sqrt{x}(1-\sqrt{x})}\right]\left[G\left(\left\{\frac{1}{\sqrt{\tau}\sqrt{1-\tau}}\right\}, x\right) - \pi\right] \quad (\text{F.8})$$

2. Integrating this expression leads to

$$F_b(x) = \frac{d}{dx}f_b(x) = \frac{1}{8}\left[G\left(\left\{\frac{1}{\sqrt{\tau}\sqrt{1-\tau}}, \frac{1}{\sqrt{\tau}\sqrt{1-\tau}}\right\}, x\right) - \pi G\left(\left\{\frac{1}{\sqrt{\tau}\sqrt{1-\tau}}\right\}, x\right)\right] - \frac{i}{8}\left[G\left(\left\{\frac{1}{\sqrt{\tau}(1-\sqrt{\tau})}, \frac{1}{\sqrt{\tau}\sqrt{1-\tau}}\right\}, x\right) - \pi G\left(\left\{\frac{1}{\sqrt{\tau}(1-\sqrt{\tau})}\right\}, x\right)\right]. \quad (\text{F.9})$$

3. & 4. Using the properties of iterated integrals and the matching

$$C = f_b(0) - F_b(0) = \text{Li}_2(1-i) = \frac{3}{8}\zeta_2 - \frac{i}{4}\pi\ln(2) - iC, \quad (\text{F.10})$$

where  $C$  denotes Catalan's constant, the final expression can be simplified to

$$\begin{aligned} f_b(x) = & \frac{1}{4}x(1-x)(1-2x)^2 + 2\sqrt{x}\sqrt{1-x}(1-2x)G(\{\sqrt{\tau}\sqrt{1-\tau}\}, x) + 4G^2(\{\sqrt{\tau}\sqrt{1-\tau}\}, x) \\ & + \frac{3}{8}\zeta_2 - \pi\left[G(\{\sqrt{\tau}\sqrt{1-\tau}\}, x) + \frac{1}{4}\sqrt{x}\sqrt{1-x}(1-2x)\right] + i\left\{\frac{1}{6}\left[1 - 6C - \sqrt{1-x}\right.\right. \\ & \left.\left. - 2x\sqrt{1-x} - 3x^{3/2}\sqrt{1-x}\right] + \frac{1}{2}G(\{\sqrt{\tau}\sqrt{1-\tau}\}, x) - G\left(\left\{\frac{1}{\sqrt{\tau}(1-\sqrt{\tau})}\right\}, x\right)\right. \\ & \left.\times G(\{\sqrt{\tau}\sqrt{1-\tau}\}, x) + G\left(\left\{\sqrt{\tau}\sqrt{1-\tau}, \frac{1}{\sqrt{\tau}(1-\sqrt{\tau})}\right\}, x\right)\right. \\ & \left. - \frac{\pi}{4}\left[\frac{1}{2}G\left(\left\{\frac{1}{\sqrt{\tau}(1-\sqrt{\tau})}\right\}, x\right) + \ln(2)\right]\right\}. \quad (\text{F.11}) \end{aligned}$$

The algorithm has been implemented in **Mathematica** and internally relies heavily on functions provided by **HarmonicSums**. This way hundreds of non-trivial polylogarithms have been reduced to their representation in iterated integrals and thereby reduced to a minimal basis. In physical quantities we have observed a not obvious cancellation of all transcendental constants except of  $\zeta$ -values.

## G. Momentum integrals in $d$ dimensions

For the direct calculation of Feynman diagrams, momentum integrals have to be performed in  $d$  dimensional space time. This appendix summarizes all steps needed in this work. In order to perform integrals in Minkowski-space the Wick-rotation is applied to all  $d$  dimensional momenta to arrive at Euclidean measures. This means the transformation

$$k_0 \rightarrow k_0^E = -ik_0 \quad (\text{G.1})$$

is applied. In the following we always assume that the Wick-rotation has been carried out and drop the superscript  $E$  for Euclidean. At the end of the calculation the Wick-rotation has to be undone for all momenta which were not integrated over.

To perform the momentum integrals, we can first combine propagators by iteratively introducing Feynman parameters via [70]

$$\frac{1}{A_1^{\alpha_1} A_2^{\alpha_2}} = \frac{\Gamma(\alpha_1 + \alpha_2)}{\Gamma(\alpha_1)\Gamma(\alpha_2)} \int_0^1 dx \frac{x^{\alpha_1-1}(1-x)^{\alpha_2-1}}{xA_1 + (1-x)A_2}. \quad (\text{G.2})$$

Subsequently symmetric integration can be used to map tensor integrals to scalar ones. In this work the following relations up to six uncontracted indices had to be used

$$\begin{aligned} \int d^d q \, q^{\mu_1} \dots q^{\mu_{2n+1}} &= 0, \\ \int d^d q \, q^{\mu_1} q^{\mu_2} f(q^2) &= \frac{g^{\mu_1 \mu_2}}{d} \int d^d q \, q^2 f(q^2), \\ \int d^d q \, q^{\mu_1} q^{\mu_2} q^{\mu_3} q^{\mu_4} f(q^2) &= \frac{S^{\mu_1 \mu_2 \mu_3 \mu_4}}{d(d+2)} \int d^d q \, q^4 f(q^2), \\ \int d^d q \, q^{\mu_1} q^{\mu_2} q^{\mu_3} q^{\mu_4} q^{\mu_5} q^{\mu_6} f(q^2) &= \frac{S^{\mu_1 \mu_2 \mu_3 \mu_4 \mu_5 \mu_6}}{d(d+2)(d+4)} \int d^d q \, q^6 f(q^2), \end{aligned} \quad (\text{G.3})$$

with the symmetric tensors

$$\begin{aligned} S^{\mu_1 \mu_2 \mu_3 \mu_4} &= g_{\mu_1 \mu_2} g_{\mu_3 \mu_4} + g_{\mu_1 \mu_3} g_{\mu_2 \mu_4} + g_{\mu_1 \mu_4} g_{\mu_2 \mu_3}, \\ S^{\mu_1 \mu_2 \mu_3 \mu_4 \mu_5 \mu_6} &= g_{\mu_1 \mu_2} [g_{\mu_3 \mu_4} g_{\mu_5 \mu_6} + g_{\mu_3 \mu_5} g_{\mu_4 \mu_6} + g_{\mu_3 \mu_6} g_{\mu_4 \mu_5}] \\ &\quad + g_{\mu_1 \mu_3} [g_{\mu_2 \mu_4} g_{\mu_5 \mu_6} + g_{\mu_2 \mu_5} g_{\mu_4 \mu_6} + g_{\mu_2 \mu_6} g_{\mu_4 \mu_5}] \\ &\quad + g_{\mu_1 \mu_4} [g_{\mu_2 \mu_3} g_{\mu_5 \mu_6} + g_{\mu_2 \mu_5} g_{\mu_3 \mu_6} + g_{\mu_2 \mu_6} g_{\mu_3 \mu_5}] \\ &\quad + g_{\mu_1 \mu_5} [g_{\mu_2 \mu_3} g_{\mu_4 \mu_6} + g_{\mu_2 \mu_4} g_{\mu_3 \mu_6} + g_{\mu_2 \mu_6} g_{\mu_3 \mu_4}] \\ &\quad + g_{\mu_1 \mu_6} [g_{\mu_2 \mu_3} g_{\mu_4 \mu_5} + g_{\mu_2 \mu_4} g_{\mu_3 \mu_5} + g_{\mu_2 \mu_5} g_{\mu_3 \mu_4}]. \end{aligned} \quad (\text{G.5})$$

This identity can be generalized to an arbitrary number of uncontracted indices

$$\int d^d q \, q^{\mu_1} \dots q^{\mu_{2n}} f(q^2) = S^{\mu_1 \dots \mu_{2n}} \frac{\Gamma(d)}{\Gamma(d+2n)} \int d^d q \, (q^2)^n f(q^2). \quad (\text{G.6})$$

Here  $f(q^2)$  can in general be any function, which only depends on  $q^2$ . However, in the context of Feynman integrals we only encounter the structure

$$f(q^2) = \frac{(q^2)^r}{(q^2 + R^2)^m}, \quad (\text{G.7})$$

with  $r$  and  $m$  positive integers. Therefore we can map all tensor integrals to the basic integral

$$\int \frac{d^d q}{(2\pi)^d} \frac{(q^2)^r}{(q^2 + R^2)^m} = \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(r + d/2)\Gamma(m - r - d/2)}{\Gamma(d/2)\Gamma(m)} (R^2)^{d/2+r-m}. \quad (\text{G.8})$$

As a special case, all scaleless diagrams vanish

$$\int \frac{d^d q}{(2\pi)^d} \frac{1}{(q^2)^m} = 0. \quad (\text{G.9})$$

After integrating over all but one loop momentum, Feynman integrals with local operator insertions additionally lead to integrals of the form

$$\int \frac{d^d q}{(2\pi)^d} (\Delta \cdot q + \Delta \cdot k)^N (q \cdot p)^n f(q^2), \quad (\text{G.10})$$

where  $k$  is a multiple of the external momentum,  $\Delta$  a light-like  $d$  dimensional vector and  $N, n \in \mathbb{N}$ . These kind of integrals can be solved by binomial decomposition

$$(\Delta \cdot q + \Delta \cdot k)^N = \sum_{j=0}^N \binom{N}{j} (\Delta \cdot q)^j (\Delta \cdot k)^{N-j} \quad (\text{G.11})$$

and applying Equation (G.6). The general formula reads

$$\int \frac{d^d q}{(2\pi)^d} (\Delta \cdot q + \Delta \cdot k)^N (q \cdot p)^n f(q^2) = \frac{\Gamma(N+1)}{\Gamma(N-n+1)} \frac{\Gamma(d)}{\Gamma(d+2n)} (\Delta \cdot k)^{N-n} (\Delta \cdot p)^n \int \frac{d^d q}{(2\pi)^d} (q^2)^n f(q^2) \quad (\text{G.12})$$

Explicitly the relations up to  $n = 3$  read

$$\int \frac{d^d q}{(2\pi)^d} (\Delta \cdot q + \Delta \cdot k)^N f(q^2) = (\Delta \cdot k)^N \int \frac{d^d q}{(2\pi)^d} f(q^2), \quad (\text{G.13})$$

$$\int \frac{d^d q}{(2\pi)^d} (\Delta \cdot q + \Delta \cdot k)^N q \cdot p f(q^2) = \frac{N}{d} (\Delta \cdot k)^{N-1} \Delta \cdot p \int \frac{d^d q}{(2\pi)^d} q^2 f(q^2), \quad (\text{G.14})$$

$$\int \frac{d^d q}{(2\pi)^d} (\Delta \cdot q + \Delta \cdot k)^N q \cdot p^2 f(q^2) = \frac{N(N-1)}{d(d+2)} (\Delta \cdot k)^{N-2} \Delta \cdot p^2 \int \frac{d^d q}{(2\pi)^d} q^4 f(q^2), \quad (\text{G.15})$$

$$\int \frac{d^d q}{(2\pi)^d} (\Delta \cdot q + \Delta \cdot k)^N q \cdot p^3 f(q^2) = \frac{N(N-1)(N-2)}{d(d+2)(d+4)} (\Delta \cdot k)^{N-3} \Delta \cdot p^3 \int \frac{d^d q}{(2\pi)^d} q^6 f(q^2). \quad (\text{G.16})$$

In deriving these relations the identities  $\Delta^2 = 0$  and  $p^2 = 0$  are crucial. This way only a single term of the binomial decomposition (G.11) survives.

For each loop integral a universal prefactor

$$S_\varepsilon = \exp \left[ \left( \gamma_E - \ln(4\pi) \right) \frac{\varepsilon}{2} \right] \quad (\text{G.17})$$

emerges, which will be kept separated and not expanded in  $\varepsilon$ . The constant  $\gamma_E$  denotes the Euler-Masceroni constant, cf. Appendix C.1. In the  $\overline{\text{MS}}$ -scheme this factor is set to one  $S_\varepsilon = 1$  at the end of the calculation and will be therefore dropped in all results presented in this thesis.

# H. Identities for Encountered Iterated Integrals

## H.1. Functions for $A_{Qq}^{(3),PS}$

To express the two-mass contributions to the OME  $A_{Qq}^{(3),PS}$  in Chapter 7.1 we introduced various iterated integrals over square root valued letters. In this section we give these quantities in terms of simple logarithmic and polylogarithmic functions at more involved arguments for which fast numeric implementations exist.

### G-functions with support $0 < x < 1$

Here, we have the argument

$$\xi_1 = x(1-x)\eta \in (0, \eta/4) \quad (\text{H.1})$$

and therefore  $\sqrt{4\xi_1 - 1} = i\sqrt{1 - 4\xi_1}$ . We also define

$$\omega_1 = \sqrt{1 - 4\xi_1}. \quad (\text{H.2})$$

We obtain:

$$G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\}, \xi_1\right) = 2\omega_1 + 2\ln(1-\omega_1) - \ln(4\xi_1) - 2 \quad (\text{H.3})$$

$$G(\{\tau|1-4\tau\}, \xi_1) = \xi_1^2 \left(\frac{1}{2} - \frac{4\xi_1}{3}\right) \quad (\text{H.4})$$

$$G(\{\tau^2|1-4\tau\}, \xi_1) = \xi_1^3 \left(\frac{1}{3} - \xi_1\right) \quad (\text{H.5})$$

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

$$\begin{aligned} G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau}\right\}, \xi_1\right) &= \omega_1(-4 - 4\ln(2) + 2\ln(4\xi_1)) \\ &\quad + \ln^2(1-\omega_1) - \frac{1}{2}\ln^2(4\xi_1) - 4\ln(1-\omega_1) \\ &\quad - 2\ln(2)\ln(1-\omega_1) + 2\ln(4\xi_1) \\ &\quad + 2\ln(2)\ln(4\xi_1) - 2\text{Li}_2\left(\frac{1-\omega_1}{2}\right) + 4 - \ln^2(2) \end{aligned} \quad (\text{H.7})$$

$$\begin{aligned} G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}\right\}, \xi_1\right) &= \omega_1(4\ln(1-\omega_1) - 4 - 2\ln(4\xi_1)) - 8\xi_1 \\ &\quad + 2\ln^2(1-\omega_1) + \frac{1}{2}\ln^2(4\xi_1) - 4\ln(1-\omega_1) \end{aligned}$$

$$G\left(\left\{\frac{1}{\tau}, \frac{1}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}\right\}, \xi_1\right) = +2\ln(4\xi_1) - 2\ln(1-\omega_1)\ln(4\xi_1) + 4 \tag{H.8}$$

$$\begin{aligned} &= 2\text{Li}_3\left(\frac{\omega_1+1}{\omega_1-1}\right) - 4\ln(1-\omega_1)\zeta_2 + 2\ln(4\xi_1)\zeta_2 \\ &+ 8\omega_1 - 2\ln^3(1-\omega_1) - \frac{1}{6}\ln^3(4\xi_1) + 2\ln^2(2) \\ &\times \ln(1-\omega_1) - 2\ln^2(1-\omega_1) + 2\ln(2) \\ &\times \ln^2(1-\omega_1) + 2\ln^2(1-\omega_1)\ln(4\xi_1) - 2\ln^2(4\xi_1) \\ &+ \ln(2)\ln^2(4\xi_1) + 8\ln(1-\omega_1) - 4\ln(2) \\ &\times \ln(1-\omega_1) - 8\ln(4\xi_1) + 4\ln(2)\ln(4\xi_1) \\ &+ 4\ln(1-\omega_1)\ln(4\xi_1) - 4\ln(2)\ln(1-\omega_1)\ln(4\xi_1) \\ &+ 4\text{Li}_2\left(\frac{1-\omega_1}{2}\right) + 4\text{Li}_3\left(\frac{1-\omega_1}{2}\right) - 8 - \frac{2}{3}\ln^3(2) \\ &- 2\ln^2(2) + 8\ln(2) \end{aligned} \tag{H.9}$$

$$\begin{aligned} G\left(\left\{\frac{1}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau}\right\}, \xi_1\right) &= (-16 - 4\ln(4\xi_1) + 2\ln^2(4\xi_1) + 8\zeta_2)\ln(1-\omega_1) \\ &+ \ln^2(1-\omega_1)(4 - 5\ln(4\xi_1)) + (12 \\ &+ 2\text{Li}_2\left(\frac{1-\omega_1}{2}\right) + 4\omega_1 - 4\zeta_2)\ln(4\xi_1) \\ &- 4\left(-4 + 2\text{Li}_2\left(\frac{1-\omega_1}{2}\right) + 2\text{Li}_3\left(\frac{1-\omega_1}{2}\right)\right) \\ &+ \text{Li}_3\left(\frac{\omega_1+1}{\omega_1-1}\right) + 4\omega_1 + \left(-8 - 4\text{Li}_2\left(\frac{1-\omega_1}{2}\right)\right) \\ &- 8\omega_1 - 2\ln^2(1-\omega_1) + 4\ln(4\xi_1) + 2\ln(1-\omega_1) \\ &\times \ln(4\xi_1) - \ln^2(4\xi_1)\ln(2) + 4\ln^3(1-\omega_1) \\ &- \frac{1}{6}\ln^3(4\xi_1) + \ln^2(2)(\ln(4\xi_1) - 4) - \frac{2}{3}\ln^3(2) \end{aligned} \tag{H.10}$$

$$\begin{aligned} G\left(\left\{\frac{1}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}, \frac{1-\sqrt{4\tau}}{\tau}\right\}, \xi_1\right) &= -(\ln(1-\omega_1)(2\ln(4\xi_1) - 4) - \ln^2(4\xi_1))\ln(2) \\ &- (2 - 2\ln(1-\omega_1) + \ln(4\xi_1))\ln^2(2) - \ln^2(1-\omega_1) \\ &\times (-5\ln(4\xi_1) - 6) - \left(8 - 4\text{Li}_2\left(\frac{1-\omega_1}{2}\right) - 8\omega_1\right) \\ &+ 8\ln(4\xi_1) + 2\ln^2(4\xi_1) + 4\zeta_2)\ln(1-\omega_1) \\ &- \left(-4 + 2\text{Li}_2\left(\frac{1-\omega_1}{2}\right) + 4\omega_1 - 2\zeta_2\right)\ln(4\xi_1) \\ &- 2\left(-4 - \text{Li}_3\left(\frac{1+\omega_1}{\omega_1-1}\right) + 2\text{Li}_2\left(\frac{1-\omega_1}{2}\right) + 4\omega_1 + 4\xi_1\right) \\ &- \frac{10}{3}\ln^3(1-\omega_1) + \frac{1}{6}\ln^3(4\xi_1) + 2\ln^2(4\xi_1) \end{aligned} \tag{H.11}$$

$$\begin{aligned} G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau}, \frac{1}{\tau}\right\}, \xi_1\right) &= 2\left(-4 + 2\text{Li}_2\left(\frac{1-\omega_1}{2}\right)\right) \\ &+ 2\text{Li}_3\left(\frac{1-\omega_1}{2}\right) + \text{Li}_3\left(\frac{1+\omega_1}{\omega_1-1}\right) + 4\omega_1 \end{aligned}$$

$$\begin{aligned}
 & + \left( 4\text{Li}_2 \left( \frac{1-\omega_1}{2} \right) + 8\omega_1 + \ln(1-\omega_1)(4-2\ln(4\xi_1)) \right. \\
 & \left. - 4(1+\omega_1)\ln(4\xi_1) + 2\ln^2(4\xi_1) \right) \ln(2) \\
 & + (2(2\omega_1+1) + 2\ln(1-\omega_1) - 3\ln(4\xi_1))\ln^2(2) \\
 & + (8 - \ln^2(4\xi_1) - 4\zeta_2)\ln(1-\omega_1) + \ln^2(1-\omega_1) \\
 & \times \left( 3\ln(4\xi_1) - 2 \right) + \left( -4 - 2\text{Li}_2 \left( \frac{1-\omega_1}{2} \right) - 4\omega_1 \right. \\
 & \left. + 2\zeta_2 \right) \ln(4\xi_1) + \frac{4}{3}\ln^3(2) - 2\ln^3(1-\omega_1) \\
 & + (1+\omega_1)\ln^2(4\xi_1) - \frac{1}{6}\ln^3(4\xi_1) \tag{H.12}
 \end{aligned}$$

$$\begin{aligned}
 G \left( \left\{ \frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau}, \frac{\sqrt{1-4\tau}}{\tau} \right\}, \xi_1 \right) & = 4 \left( -\text{Li}_3 \left( \frac{\omega_1+1}{\omega_1-1} \right) + \text{Li}_2 \left( \frac{1-\omega_1}{2} \right) + \text{Li}_2 \left( \frac{1-\omega_1}{2} \right) \right. \\
 & \times \omega_1 - 4\xi_1 \left. \right) - \left( (4(\omega_1-1) - 6\ln(4\xi_1))\ln(1-\omega_1) \right. \\
 & \left. - 8(\omega_1-1) + 4\ln^2(1-\omega_1) + 4\ln(4\xi_1) + 2\ln^2(4\xi_1) \right) \\
 & \times \ln(2) - (-2(1+\omega_1) + 2\ln(1-\omega_1) - \ln(4\xi_1))\ln^2(2) \\
 & - \left( -\ln^2(4\xi_1) + 4\text{Li}_2 \left( \frac{1-\omega_1}{2} \right) - 8\zeta_2 \right. \\
 & \left. - 4\ln(4\xi_1)\omega_1 \right) \ln(1-\omega_1) - \left( 2(1+\omega_1) \right. \\
 & \left. + 5\ln(4\xi_1) \right) \ln^2(1-\omega_1) - \left( -4 - 2\text{Li}_2 \left( \frac{1-\omega_1}{2} \right) \right. \\
 & \left. + 4\omega_1 + 4\zeta_2 \right) \ln(4\xi_1) + \frac{14}{3}\ln^3(1-\omega_1) \\
 & - (\omega_1-1)\ln^2(4\xi_1) + \frac{1}{6}\ln^3(4\xi_1) \tag{H.13}
 \end{aligned}$$

$$\begin{aligned}
 G \left( \left\{ \frac{\sqrt{1-4\tau}}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau} \right\}, \xi_1 \right) & = \left( 8 - 4\ln^2(2) - 2\zeta_2 - 4\ln(2)\omega_1 \right) \ln(4\xi_1) \\
 & + \left[ -4(1+2\xi_1+\omega_1) + 6\ln^2(2) - 4\ln(4\xi_1) \right. \\
 & \left. + \ln^2(4\xi_1) + 4\ln^2(\omega_1+1) + 4\zeta_2 + \ln(1+\omega_1) \right. \\
 & \left. \times (-4\omega_1 - 8\ln(2)) + 4\ln(2)(1+\omega_1) \right] \ln(1-\omega_1) \\
 & + \left( 4(-3-2\xi_1+\omega_1) + 10\ln^2(2) + 4\ln(2)(2\omega_1+1) \right) \\
 & \times \ln(1+\omega_1) + \left( -4\ln(2) + 4\ln(\omega_1+1) - 4\omega_1 \right) \\
 & \times \text{Li}_2 \left( \frac{1-\omega_1}{2} \right) + 4\zeta_2 + 4\zeta_3 + 8(3\xi_1+\omega_1-1) \\
 & + \left( 2 - 2\ln(4\xi_1) - 2\ln(2) \right) \ln^2(1-\omega_1) + \ln^2(4\xi_1) \\
 & \times \left( \omega_1 + 2\ln(2) + 1 \right) - \frac{1}{2}\ln^3(4\xi_1) + 16\ln(2)\xi_1 \\
 & - 4\text{Li}_2 \left( \frac{1-\omega_1}{2} \right) - 2\text{Li}_3 \left( \frac{\omega_1+1}{\omega_1-1} \right) - 4\text{Li}_3 \left( \frac{1-\omega_1}{2} \right)
 \end{aligned}$$

$$\begin{aligned}
 & -4\text{Li}_3\left(\frac{1+\omega_1}{2}\right) + \left(4\ln(1+\omega_1) - 4\ln(2) - 4\right) \\
 & \text{Li}_2\left(\frac{1+\omega_1}{2}\right) + 2\ln^3(1-\omega_1) + \frac{2}{3}\ln^3(1+\omega_1) \\
 & -\left(2(1+\omega_1) + 6\ln(2)\right)\ln^2(\omega_1+1) - 2\ln^2(2) \\
 & \times(\omega_1+2) - \frac{8}{3}\ln^3(2).
 \end{aligned} \tag{H.14}$$

**G-functions with support**  $x \in [0, \frac{1}{2} - \frac{1}{2}\sqrt{1-\eta}] \cup [\frac{1}{2} + \frac{1}{2}\sqrt{1-\eta}, 1]$

The integrals in this class coincide with integrals with full support ( $0 < x < 1$ ), but the replacements

$$\xi_1 \rightarrow \xi_3 = \frac{x(1-x)}{\eta}, \tag{H.15}$$

$$\omega_1 \rightarrow \omega_3 = \sqrt{1-4\xi_3} \tag{H.16}$$

have to be performed.

**G-functions with support**  $\frac{1}{2} - \frac{1}{2}\sqrt{1-\eta} < x < \frac{1}{2} + \frac{1}{2}\sqrt{1-\eta}$

Here, we have the argument

$$\xi_2 = \frac{\eta}{x(1-x)} \in (4\eta, 4) \tag{H.17}$$

and therefore  $\sqrt{4-\xi_2}$  is real. We introduce the abbreviations

$$\omega_2 = \sqrt{\xi_2}\sqrt{4-\xi_2}, \tag{H.18}$$

$$\phi = \arcsin\left(\frac{\sqrt{\xi_2}}{2}\right). \tag{H.19}$$

$$G\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\}, \xi_2\right) = -\omega_2\left(1 - \frac{\xi_2}{2}\right) + 4\phi \tag{H.20}$$

$$\begin{aligned}
 G\left(\left\{\frac{1}{4-\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, \xi_2\right) &= -\frac{1}{2}\omega_2\left(1 + \frac{\xi_2}{2}\right) + \left(2 - 4\ln(4-\xi_2)\right)\phi \\
 &+ 4\text{Cl}_2(2\phi) - 2\text{Cl}_2(4\phi)
 \end{aligned} \tag{H.21}$$

$$\begin{aligned}
 G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, \xi_2\right) &= \omega_2\left(\frac{\xi_2}{4} - \frac{3}{2}\right) - \left(2 - 4\ln(\xi_2)\right)\phi + 4\text{Cl}_2(2\phi) \\
 &+ 8\text{Cl}_2(4\phi)
 \end{aligned} \tag{H.22}$$

$$\begin{aligned}
 G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, \xi_2\right) &= 5\xi_2 - \frac{3}{2}\xi_2^2 + \frac{1}{3}\xi_2^3 - \frac{1}{32}\xi_2^4 - 8\zeta_3 + \phi\left[(\xi_2 - 6)\omega_2\right. \\
 &\left.+ 16\text{Cl}_2(2\phi)\right] + 8\text{Cl}_3(2\phi) + \phi^2(8\ln(\xi_2) - 4).
 \end{aligned} \tag{H.23}$$

We used the Clausen function [265, 266]

$$\begin{aligned}
 \text{Cl}_2(x) &= \frac{i}{2}(\text{Li}_2(e^{-ix}) - \text{Li}_2(e^{ix})), \\
 \text{Cl}_3(x) &= \frac{1}{2}(\text{Li}_3(e^{-ix}) + \text{Li}_3(e^{ix}))
 \end{aligned} \tag{H.24}$$



with the sum representation

$$\begin{aligned} \text{Cl}_2(\phi) &= \sum_{n=1}^{\infty} \frac{\sin(n\phi)}{n^2}, \\ \text{Cl}_3(\phi) &= \sum_{n=1}^{\infty} \frac{\cos(n\phi)}{n^3} \end{aligned} \quad (\text{H.25})$$

for  $\phi \in (0, 2\pi)$ .

## H.2. Functions for $A_{gg,Q}^{(3)}$

Before the absorption of a few rational pre-factors in  $N$ , all emerging integrals first written in  $G$ -functions in Chapter 7.2 can be expressed in terms of polylogarithms at algebraic arguments in  $z$  and  $\eta$ . In cases it leads to simplifications, we also use arcus- and area-functions instead of logarithms, which belong to the harmonic (poly)logarithms of complex-valued argument.

The different functions  $G_l \equiv G_l(z, \eta)$  and constants  $K_l = K_l(\eta)$  are given by

$$G_1 = G \left[ \left\{ \sqrt{(1-x)x} \right\}, z \right] = \frac{1}{2} \sqrt{1-z} z^{3/2} - \frac{1}{4} \sqrt{1-z} \sqrt{z} - \frac{1}{4} \arctan \left( \frac{\sqrt{1-z}}{\sqrt{z}} \right) + \frac{\pi}{8} \quad (\text{H.26})$$

$$G_2 = G \left[ \left\{ \frac{1}{z + \eta(1-x)} \right\}, z \right] = \frac{\ln(z + \eta(1-z)) - \ln(\eta)}{1 - \eta} \quad (\text{H.27})$$

$$G_3 = G \left[ \left\{ \frac{1}{1-z(1-\eta)} \right\}, z \right] = -\frac{\ln(1-z(1-\eta))}{1-\eta} \quad (\text{H.28})$$

$$\begin{aligned} G_4 = G \left[ \left\{ \frac{\sqrt{x(1-x)}}{1-x(1-\eta)} \right\}, z \right] &= \frac{1}{(1-\eta)^2} \left[ \frac{1}{2} \pi(\eta+1) - (1-\eta) \sqrt{(1-z)z} \right. \\ &\quad \left. - (\eta+1) \arctan \left( \frac{\sqrt{1-z}}{\sqrt{z}} \right) - 2\sqrt{\eta} \arctan \left( \frac{\sqrt{\eta}\sqrt{z}}{\sqrt{1-z}} \right) \right] \end{aligned} \quad (\text{H.29})$$

$$\begin{aligned} G_5 = G \left[ \left\{ -\frac{\sqrt{x(1-x)}}{x(1-\eta) + \eta} \right\}, z \right] &= \frac{1}{(1-\eta)^2} \left[ -\frac{\pi}{2}(1+\eta) - \sqrt{z(1-z)}(1-\eta) \right. \\ &\quad \left. + 2\sqrt{\eta} \arctan \left( \frac{\sqrt{z}}{\sqrt{(1-z)\eta}} \right) + (1+\eta) \arctan \left( \frac{\sqrt{1-z}}{\sqrt{z}} \right) \right] \end{aligned} \quad (\text{H.30})$$

$$\begin{aligned} G_6 = G \left[ \left\{ \sqrt{(1-x)x}, \frac{1}{1-x} \right\}, z \right] &= \frac{1}{4} \ln(1-z) \sqrt{(1-z)z} (1-2z) + \left[ \arcsin(\sqrt{1-z}) \right. \\ &\quad \left. - \frac{1}{4} i \ln(1-z) \right] \ln(i\sqrt{1-z} + \sqrt{z}) - \frac{1}{2} \arcsin(\sqrt{1-z}) \ln \left( -1 + (\sqrt{z} + i\sqrt{1-z})^2 \right) \\ &\quad + \frac{1}{48} \left[ -3\pi + 6 \arcsin(\sqrt{1-z}) - 12i \arcsin^2(\sqrt{1-z}) + 6\sqrt{(1-z)z}(1+2z) \right. \\ &\quad \left. + 12i\zeta_2 - 12i \text{Li}_2 \left( \frac{1}{(i\sqrt{1-z} + \sqrt{z})^2} \right) \right] + \frac{1}{4} \pi \ln(2) \end{aligned} \quad (\text{H.31})$$

$$G_7 = G \left[ \left\{ \sqrt{(1-x)x}, \frac{1}{x} \right\}, z \right] = \frac{i}{2} \text{Li}_2(-\sqrt{1-z} - i\sqrt{z}) - \frac{i}{2} \text{Li}_2(1 - \sqrt{1-z} - i\sqrt{z})$$

$$\begin{aligned}
 & + \ln(z) \left( \frac{1}{2} \sqrt{1-z} z^{3/2} - \frac{1}{4} \sqrt{(1-z)z} + \frac{1}{4} \arcsin(\sqrt{z}) \right) \\
 & + \frac{3}{8} \sqrt{1-z} \sqrt{z} + \frac{i}{4} \arctan^2 \left( \frac{\sqrt{z}}{\sqrt{1-z}} \right) + \arctan \left( \frac{\sqrt{z}}{\sqrt{1-z}} \right) \\
 & \times \left( \frac{1}{8} - \frac{1}{2} \ln(\sqrt{1-z} + i\sqrt{z} + 1) \right) + \frac{i\zeta_2}{4} - \frac{1}{4} \sqrt{1-z} z^{3/2}
 \end{aligned} \tag{H.32}$$

$$\begin{aligned}
 G_8 = G \left[ \left\{ \frac{1}{x + \eta(1-x)}, \frac{1}{1-x} \right\}, z \right] &= -\frac{1}{1-\eta} \left[ \ln(1-z) \ln(z + \eta(1-z)) \right. \\
 & \left. + \text{Li}_2((1-\eta)(1-z)) - \text{Li}_2((1-\eta)) \right]
 \end{aligned} \tag{H.33}$$

$$\begin{aligned}
 G_9 = G \left[ \left\{ \frac{1}{x + \eta(1-x)}, \frac{1}{x} \right\}, z \right] &= \frac{1}{1-\eta} \left[ \text{Li}_2 \left( -\frac{z(1-\eta)}{\eta} \right) + \ln(z) (\ln((1-\eta)z + \eta) \right. \\
 & \left. - \ln(\eta)) \right]
 \end{aligned} \tag{H.34}$$

$$\begin{aligned}
 G_{10} = G \left[ \left\{ \frac{1}{1-x(1-\eta)}, \frac{1}{1-x} \right\}, z \right] &= \frac{1}{1-\eta} \left[ \text{Li}_2 \left( -\frac{(1-z)(1-\eta)}{\eta} \right) \right. \\
 & \left. + \ln(1-z) (\ln(1 - (1-\eta)z) - \ln(\eta)) - \text{Li}_2 \left( -\frac{1-\eta}{\eta} \right) \right]
 \end{aligned} \tag{H.35}$$

$$G_{11} = G \left[ \left\{ \frac{1}{1-x(1-\eta)}, \frac{1}{x} \right\}, z \right] = -\frac{1}{1-\eta} \left[ \ln(z) \ln(1-z(1-\eta)) + \text{Li}_2(z(1-\eta)) \right] \tag{H.36}$$

$$\begin{aligned}
 G_{12} = G \left[ \left\{ \frac{\sqrt{(1-x)x}}{1-x(1-\eta)}, \frac{1}{1-x} \right\}, z \right] &= \frac{1}{(1-\eta)^2} \left[ -i \left[ \eta \text{Li}_2 \left( -(\sqrt{1-z} + i\sqrt{z})^2 \right) \right. \right. \\
 & + \sqrt{\eta} \text{Li}_2 \left( \frac{\left(1 - \frac{i\sqrt{z}}{\sqrt{1-z}}\right) \sqrt{\eta}}{\sqrt{\eta} - 1} \right) - \sqrt{\eta} \text{Li}_2 \left( \frac{\left(\frac{i\sqrt{z}}{\sqrt{1-z}} + 1\right) \sqrt{\eta}}{\sqrt{\eta} - 1} \right) \\
 & - \sqrt{\eta} \text{Li}_2 \left( \frac{\left(1 - \frac{i\sqrt{z}}{\sqrt{1-z}}\right) \sqrt{\eta}}{\sqrt{\eta} + 1} \right) + \sqrt{\eta} \text{Li}_2 \left( \frac{\left(\frac{i\sqrt{z}}{\sqrt{1-z}} + 1\right) \sqrt{\eta}}{\sqrt{\eta} + 1} \right) \\
 & \left. + \text{Li}_2 \left( -(\sqrt{1-z} + i\sqrt{z})^2 \right) \right] + (\eta - 1) \sqrt{(1-z)z} + i(\eta + 1) \arcsin^2(\sqrt{z}) \\
 & + (1-\eta) \arcsin(\sqrt{z}) + 2(\eta + 1) \ln(2) \arcsin(\sqrt{z}) \\
 & + \ln(1-z) \left[ (1-\eta) \sqrt{(1-z)z} + 2\sqrt{\eta} \arctan \left( \frac{\sqrt{\eta z}}{\sqrt{1-z}} \right) \right] + \ln \left( \frac{1-\sqrt{\eta}}{\sqrt{\eta} + 1} \right) (\pi\sqrt{\eta} \\
 & - 2\sqrt{\eta} \arctan \left( \frac{\sqrt{1-z}}{\sqrt{z}} \right)) - \frac{1}{2} i(\eta + 1) \zeta_2 \right]
 \end{aligned} \tag{H.37}$$

$$G_{13} = G \left[ \left\{ \frac{\sqrt{(1-x)x}}{1-x(1-\eta)}, \frac{1}{x} \right\}, z \right] = -\frac{i(1+\eta)\pi \arcsin(\sqrt{z})}{(1-\eta)^2} - i \frac{(1+\eta) \arcsin(\sqrt{z})^2}{(1-\eta)^2}$$

$$\begin{aligned}
 & -\frac{2(1+\eta)\arcsin(\sqrt{z})\ln(2)}{(1-\eta)^2} + \frac{1}{(1-\eta)^2} \left[ -i(1+\eta)\text{Li}_2\left(\frac{1}{(\sqrt{1-z}+i\sqrt{z})^2}\right) \right. \\
 & + (1-\eta)\sqrt{(1-z)z} + (1+\eta)i\zeta_2 + 2i\sqrt{\eta}\text{Li}_2\left(-\frac{i\sqrt{\eta}\sqrt{z}}{\sqrt{1-z}}\right) - 2i\sqrt{\eta}\text{Li}_2\left(\frac{i\sqrt{\eta}\sqrt{z}}{\sqrt{1-z}}\right) \\
 & + i\sqrt{\eta}\text{Li}_2\left(\frac{\sqrt{\eta}(1-\frac{i\sqrt{z}}{\sqrt{1-z}})}{-1+\sqrt{\eta}}\right) - i\sqrt{\eta}\text{Li}_2\left(\frac{\sqrt{\eta}(1-\frac{i\sqrt{z}}{\sqrt{1-z}})}{1+\sqrt{\eta}}\right) - i\sqrt{\eta}\text{Li}_2\left(\frac{\sqrt{\eta}(1+\frac{i\sqrt{z}}{\sqrt{1-z}})}{-1+\sqrt{\eta}}\right) \\
 & \left. + i\sqrt{\eta}\text{Li}_2\left(\frac{\sqrt{\eta}(1+\frac{i\sqrt{z}}{\sqrt{1-z}})}{1+\sqrt{\eta}}\right) \right] + \arctan\left(\frac{\sqrt{1-z}}{\sqrt{z}}\right) \left[ \frac{4\ln(1-\sqrt{\eta})}{(1-\eta)^2}\sqrt{\eta} - \frac{2\sqrt{\eta}\ln(1-\eta)}{(1-\eta)^2} \right] \\
 & + \arctan\left(\frac{\sqrt{z}}{\sqrt{1-z}}\right) \left[ \frac{1}{1-\eta} + \frac{2i(1+\eta)\arcsin(\sqrt{z})}{(1-\eta)^2} + \frac{(1+\eta)\ln(z)}{(1-\eta)^2} \right] \\
 & - \frac{2\pi\ln(1-\sqrt{\eta})}{(1-\eta)^2}\sqrt{\eta} - \frac{2\ln(z)}{(1-\eta)^2} \left( \arctan\left(\frac{\sqrt{\eta}\sqrt{z}}{\sqrt{1-z}}\right) \right) \sqrt{\eta} + \frac{\pi\sqrt{\eta}\ln(1-\eta)}{(1-\eta)^2} \\
 & - \left[ \frac{(1+\eta)\arcsin(\sqrt{z})}{(1-\eta)^2} + \frac{\sqrt{(1-z)z}}{1-\eta} \right] \ln(z), \tag{H.38}
 \end{aligned}$$

$$\begin{aligned}
 G_{14} & = G \left[ \left\{ -\frac{\sqrt{(1-x)x}}{x(1-\eta)+\eta}, \frac{1}{1-x} \right\}, z \right] = -\frac{(1+\eta)\ln(2)\pi}{(1-\eta)^2} + i\frac{(1+\eta)\arcsin(\sqrt{1-z})^2}{(1-\eta)^2} \\
 & + \frac{1}{(-1+\eta)^2} \left[ \frac{1}{2}(1-\eta)\pi + i\eta\text{Li}_2\left(-\frac{1}{1-2z-2i\sqrt{(1-z)z}}\right) - (1-\eta)\frac{\sqrt{z}}{\sqrt{1-z}} \right. \\
 & + (1-\eta)\frac{z^{3/2}}{\sqrt{1-z}} - i(1+\eta)\zeta_2 + i\sqrt{\eta}\text{Li}_2\left(\frac{1-\frac{i\sqrt{z}}{\sqrt{1-z}}}{1-\sqrt{\eta}}\right) - i\sqrt{\eta}\text{Li}_2\left(\frac{1-\frac{i\sqrt{z}}{\sqrt{1-z}}}{1+\sqrt{\eta}}\right) \\
 & \left. - i\sqrt{\eta}\text{Li}_2\left(\frac{1+\frac{i\sqrt{z}}{\sqrt{1-z}}}{1-\sqrt{\eta}}\right) + i\sqrt{\eta}\text{Li}_2\left(\frac{1+\frac{i\sqrt{z}}{\sqrt{1-z}}}{1+\sqrt{\eta}}\right) + i\text{Li}_2\left(-\frac{1}{1-2z-2i\sqrt{(1-z)z}}\right) \right] \\
 & + \frac{1+\eta}{(1-\eta)^2}\arcsin(\sqrt{1-z}) \left[ 2\ln(2) + i\pi \right] + \frac{2\sqrt{\eta}}{(1-\eta)^2}\arctan\left(\frac{\sqrt{z}}{\sqrt{1-z}}\right) \left[ -i\pi \right. \\
 & \left. - 2\ln(1-\sqrt{\eta}) + \ln(1-\eta) \right] + \arctan\left(\frac{\sqrt{1-z}}{\sqrt{z}}\right) \left[ -\frac{1}{1-\eta} - i\frac{2(1+\eta)\arcsin(\sqrt{1-z})}{(1-\eta)^2} \right. \\
 & \left. - \frac{(1+\eta)\ln(1-z)}{(1-\eta)^2} \right] + \frac{2\pi\ln(1-\sqrt{\eta})}{(1-\eta)^2}\sqrt{\eta} - \frac{2\sqrt{\eta}\ln(1-z)}{(1-\eta)^2}\arctan\left(\frac{\sqrt{z}}{\sqrt{\eta}\sqrt{1-z}}\right) \\
 & - \frac{2\sqrt{\eta}\pi}{(1-\eta)^2}\ln\left(1-\frac{i\sqrt{z}}{\sqrt{1-z}}\right) + \left[ \frac{(1+\eta)\arcsin(\sqrt{1-z})}{(1-\eta)^2} + \frac{\sqrt{(1-z)z}}{1-\eta} \right] \ln(1-z), \tag{H.39}
 \end{aligned}$$

$$\begin{aligned}
 G_{15} & = G \left[ \left\{ -\frac{\sqrt{(1-x)x}}{\eta+x(1-\eta)}, \frac{1}{x} \right\}, z \right] = -i\frac{(1+\eta)\arcsin^2(\sqrt{z})}{(1-\eta)^2} + \frac{1}{6(1-\eta)^2} \left[ 3(1-\eta)\pi \right. \\
 & - 6i\eta\text{Li}_2(1-2z+2i\sqrt{(1-z)z}) + 6(1-\eta)\sqrt{(1-z)z} + 6(1-6\sqrt{\eta}+\eta)i\zeta_2 \\
 & \left. - 12i\sqrt{\eta}\text{Li}_2\left(-\frac{i\sqrt{z}}{\sqrt{\eta}\sqrt{1-z}}\right) + 12i\sqrt{\eta}\text{Li}_2\left(\frac{i\sqrt{z}}{\sqrt{\eta}\sqrt{1-z}}\right) + 6i\sqrt{\eta}\text{Li}_2\left(\frac{1-\frac{i\sqrt{z}}{\sqrt{1-z}}}{1+\sqrt{\eta}}\right) \right]
 \end{aligned}$$

$$\begin{aligned}
 & +6i\sqrt{\eta}\text{Li}_2\left(\frac{1+\frac{i\sqrt{z}}{\sqrt{1-z}}}{1-\sqrt{\eta}}\right) - 6i\sqrt{\eta}\text{Li}_2\left(\frac{1+\frac{i\sqrt{z}}{\sqrt{1-z}}}{1+\sqrt{\eta}}\right) - 6i\sqrt{\eta}\text{Li}_2\left(\frac{i(i+\frac{\sqrt{z}}{\sqrt{1-z}})}{-1+\sqrt{\eta}}\right) \\
 & -6i\text{Li}_2\left(1-2z+2i\sqrt{(1-z)z}\right) + \frac{1+\eta}{(1-\eta)^2} \arcsin(\sqrt{z}) \left[2\ln(2) - i\pi\right] \\
 & + \frac{2}{(1-\eta)^2} \arctan\left(\frac{\sqrt{z}}{\sqrt{1-z}}\right) \left[i(1+\eta) \arcsin(\sqrt{z}) + i\pi\sqrt{\eta} + 2\sqrt{\eta} \ln(1-\sqrt{\eta})\right. \\
 & \left. - \sqrt{\eta} \ln(1-\eta)\right] + \frac{1}{(1-\eta)^2} \arctan\left(\frac{\sqrt{1-z}}{\sqrt{z}}\right) \left[-1+\eta + 2i\sqrt{\eta}\pi + (1+\eta) \ln(z)\right] \\
 & - \frac{2\pi}{(1-\eta)^2} \sqrt{\eta} \ln(1-\sqrt{\eta}) + \frac{2\sqrt{\eta}}{(1-\eta)^2} \ln(z) \arctan\left(\frac{\sqrt{z}}{\sqrt{\eta}\sqrt{1-z}}\right) - \frac{\pi\sqrt{\eta} \ln(1-z)}{(1-\eta)^2} \\
 & + \frac{1}{(1-\eta)^2} \left[(1+\eta) \arcsin(\sqrt{z}) + \frac{1}{2}(- (1+\eta)\pi + 2(-1+\eta)\sqrt{(1-z)z})\right] \ln(z). \quad (\text{H.40})
 \end{aligned}$$

Furthermore, the functions  $K_l(\eta) \equiv K_l$  contribute. For the more complicated among them we first obtained a longer representation, which finally could be reduced. In these cases we present both representations, since they contain relations between polylogarithms. Structures like this are particularly obtained by integrating using **Mathematica**. The comparison of both these cases may be helpful in other calculations to obtain more compact results.

$$\begin{aligned}
 K_1 &= G\left[\left\{\sqrt{(1-\eta-x)x}\right\}, 1\right] = \frac{1}{8}(1-\eta)^2\pi + \frac{i}{8}\left[2(1+\eta)\sqrt{\eta} - 2(1-\eta)^2 \ln(1+\sqrt{\eta})\right. \\
 & \left. + (1-\eta)^2 \ln(1-\eta)\right] \quad (\text{H.41})
 \end{aligned}$$

$$K_2 = G\left[\left\{\frac{1}{\eta+x(1-\eta)}\right\}, 1\right] = -\frac{\ln(\eta)}{1-\eta} \quad (\text{H.42})$$

$$K_3 = G\left[\left\{\frac{1}{1-\eta(1-x)}\right\}, 1\right] = -\frac{\ln(1-\eta)}{\eta} \quad (\text{H.43})$$

$$K_4 = G\left[\left\{\sqrt{x(1-\eta(1-x))}\right\}, 1\right] = \frac{(1-\eta)^2}{8\eta^{3/2}} \left[\ln(1-\eta) - 2\ln(1+\sqrt{\eta})\right] + \frac{1+\eta}{4\eta} \quad (\text{H.44})$$

$$K_5 = G\left[\left\{\frac{1}{1-x(1-\eta)}\right\}, 1\right] = -\frac{\ln(\eta)}{1-\eta} \quad (\text{H.45})$$

$$K_6 = G\left[\left\{\frac{\sqrt{(1-x)x}}{1-x(1-\eta)}\right\}, 1\right] = \frac{\pi}{2(1+\sqrt{\eta})^2} \quad (\text{H.46})$$

$$K_7 = G\left[\left\{-\frac{\sqrt{(1-x)x}}{x(1-\eta)+\eta}\right\}, 1\right] = -\frac{\pi}{2(1+\sqrt{\eta})^2} \quad (\text{H.47})$$

$$K_8 = G\left[\left\{\frac{1}{\eta(1-x)+x}, \frac{1}{1-x}\right\}, 1\right] = \frac{\text{Li}_2(1-\eta)}{1-\eta} \quad (\text{H.48})$$

$$K_9 = G\left[\left\{\frac{1}{\eta+x(1-\eta)}, \frac{1}{x}\right\}, 1\right] = -\frac{\frac{1}{2}\ln^2(\eta) + \text{Li}_2(1-\eta)}{1-\eta} \quad (\text{H.49})$$

$$\begin{aligned}
 K_{10} &= G\left[\left\{\sqrt{x(1-\eta(1-x))}, \frac{1}{1-\eta(1-x)}\right\}, 1\right] = \frac{(1-\eta)^2}{\eta^{5/2}} \left[\frac{1}{8}\ln^2(1-\sqrt{\eta})\right. \\
 & \left. - \frac{\ln(1-\eta)}{16(1-\eta)^2}(1+4\sqrt{\eta}-2\eta+4\eta^{3/2}+\eta^2) - \frac{1}{8}\zeta_2 + \frac{(1-3\eta)\sqrt{\eta}}{8(1-\eta)^2} - \frac{1}{4}\text{Li}_2\left(\frac{1}{2}(1+\sqrt{\eta})\right)\right]
 \end{aligned}$$

$$\begin{aligned}
 & - \left[ \frac{3}{8} \ln(\sqrt{2}-1) + \frac{1}{4} \ln(1-\sqrt{\eta}) - \frac{1}{4} \ln(1-\eta) \right] \ln(2) + \frac{5 \ln^2(2)}{32} - \frac{3}{8} \ln^2(\sqrt{2}-1) \\
 & + \frac{1}{16} \ln^2(1-\eta) + \ln(1-\sqrt{\eta}) \left[ \frac{1}{8} - \frac{1}{4} \ln(1-\eta) \right] + \frac{1}{4} \text{Li}_2 \left( \frac{1}{2} \left( 1 + \frac{1}{\sqrt{2}} \right) \right) \\
 & - \frac{1}{4} \text{Li}_2 \left( -(\sqrt{2}-1)^2 \right) \quad (H.50)
 \end{aligned}$$

$$K_{11} = G \left[ \left\{ \frac{1}{1-x(1-\eta)}, \frac{1}{1-x} \right\}, 1 \right] = \frac{1}{1-\eta} \left[ \frac{1}{2} \ln^2(\eta) - \ln(1-\eta) \ln(\eta) - \text{Li}_2(\eta) + \zeta_2 \right] \quad (H.51)$$

$$K_{12} = G \left[ \left\{ \frac{1}{1-x(1-\eta)}, \frac{1}{x} \right\}, 1 \right] = -\frac{\text{Li}_2(1-\eta)}{1-\eta} \quad (H.52)$$

$$\begin{aligned}
 K_{13} = G \left[ \left\{ \frac{\sqrt{(1-x)x}}{1-x(1-\eta)}, \frac{1}{1-x} \right\}, 1 \right] &= \frac{\pi}{(1-\eta)^2} \left[ \frac{1}{2} (1-\eta) - \sqrt{\eta} [2 \ln(\sqrt{\eta}+1) \right. \\
 & \left. - \ln(\eta)] + (\eta+1) \ln(2) \right] \quad (H.53)
 \end{aligned}$$

$$K_{14} = G \left[ \left\{ \frac{\sqrt{(1-x)x}}{1-x(1-\eta)}, \frac{1}{x} \right\}, 1 \right] = \frac{\pi}{(1-\eta)^2} \left[ \frac{1-\eta}{2} - (1+\eta) \ln(2) + 2\sqrt{\eta} \ln(\sqrt{\eta}+1) \right] \quad (H.54)$$

$$\begin{aligned}
 K_{15} = G \left[ \left\{ \frac{\sqrt{(1-x)x}}{1-x(1-\eta)}, \sqrt{(1-x)x} \right\}, 1 \right] &= \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ \frac{1+\eta+\eta^2}{6(1-\eta)\sqrt{\eta}} + \frac{3-5\sqrt{\eta}+3\eta}{16} \frac{\zeta_2}{\sqrt{\eta}} \right. \\
 & - \frac{1}{16} \ln^2(2) + \frac{1}{4} \ln(2) \ln(\sqrt{2}-1) - \left[ \frac{1}{8} \ln(1-\eta) - \frac{1}{4} \ln(1-\sqrt{\eta}) - \frac{(1+\eta)\sqrt{\eta}}{4(\eta-1)^2} \right] \ln(\eta) \\
 & \left. - \frac{1}{2} \text{Li}_2 \left( \frac{1}{\sqrt{2}} \right) - \frac{1}{2} \text{Li}_2 \left( (\sqrt{2}-1)^2 \right) + \frac{1}{8} \text{Li}_2 \left( (\sqrt{2}-1)^4 \right) + \frac{\text{Li}_2(\sqrt{\eta})}{2} - \frac{\text{Li}_2(\eta)}{8} \right] \quad (H.55)
 \end{aligned}$$

$$\begin{aligned}
 K_{16} = G \left[ \left\{ \frac{\sqrt{(1-x)x}}{-\eta-x(1-\eta)}, \frac{1}{1-x} \right\}, 1 \right] &= -\frac{\pi}{(1-\eta)^2} \left[ \frac{\eta-1}{2} + (1+\eta) \ln(2) \right. \\
 & \left. - 2\sqrt{\eta} \ln(\sqrt{\eta}+1) \right] \quad (H.56)
 \end{aligned}$$

$$\begin{aligned}
 K_{17} = G \left[ \left\{ -\frac{\sqrt{(1-x)x}}{\eta+x(1-\eta)}, \frac{1}{x} \right\}, 1 \right] &= \frac{\pi}{(1-\eta)^2} \left[ \frac{1-\eta}{2} - 2\sqrt{\eta} \ln(\sqrt{\eta}+1) + \sqrt{\eta} \ln(\eta) \right. \\
 & \left. + (\eta+1) \ln(2) \right] \quad (H.57)
 \end{aligned}$$

$$\begin{aligned}
 K_{18} = G \left[ \left\{ -\frac{\sqrt{(1-x)x}}{x+\eta(1-x)}, \sqrt{(1-x)x} \right\}, 1 \right] &= \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ \frac{(1+\eta+\eta^2)}{6(1-\eta)\sqrt{\eta}} - \frac{3-7\sqrt{\eta}+3\eta}{16} \frac{\zeta_2}{\sqrt{\eta}} \right. \\
 & - \frac{1}{16} \ln^2(2) + \frac{1}{4} \ln(2) \ln(\sqrt{2}-1) + \left[ \frac{(1+\eta)\sqrt{\eta}}{4(1-\eta)^2} - \frac{1}{4} \ln(1+\sqrt{\eta}) + \frac{1}{8} \ln(1-\eta) \right] \ln(\eta) \\
 & \left. - \frac{1}{2} \text{Li}_2 \left( \frac{1}{\sqrt{2}} \right) - \frac{1}{2} \text{Li}_2 \left( (\sqrt{2}-1)^2 \right) + \frac{1}{8} \text{Li}_2 \left( (\sqrt{2}-1)^4 \right) + \frac{\text{Li}_2(\sqrt{\eta})}{2} - \frac{\text{Li}_2(\eta)}{8} \right]
 \end{aligned}$$

(H.58)

$$K_{19} = G \left[ \left\{ \sqrt{(1-x)x}, \sqrt{(1-x)x}, \frac{1}{1-x} \right\}, 1 \right] = \frac{7}{192} - \frac{3}{128}\zeta_2 - \frac{7}{128}\zeta_3 + \frac{3}{32} \ln(2)\zeta_2 \quad (\text{H.59})$$

$$K_{20} = G \left[ \left\{ \sqrt{(1-x)x}, \sqrt{(1-x)x}, \frac{1}{x} \right\}, 1 \right] = \frac{7}{192} + \frac{3}{128}\zeta_2 - \frac{7}{128}\zeta_3 - \frac{3}{32} \ln(2)\zeta_2 \quad (\text{H.60})$$

$$\begin{aligned} K_{21} &= G \left[ \left\{ \frac{\sqrt{(1-x)x}}{1-x(1-\eta)}, \frac{1}{1-x}, \sqrt{(1-x)x} \right\}, 1 \right] \\ &= \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ \frac{1}{8} (2i\pi + 3 \ln(\eta)) \ln^2(1-\sqrt{\eta}) - \frac{1}{4} \ln(2) \text{Li}_2 \left( \frac{1}{2} \left( 1 + \frac{1}{\sqrt{2}} \right) \right) \right. \\ &\quad - \frac{1}{4} \ln(\eta) \text{Li}_2 \left( \frac{1}{2} (1 + \sqrt{\eta}) \right) + \frac{1}{4} (1 + 2 \ln(\eta)) \text{Li}_2(\sqrt{\eta}) - \frac{1}{2} \text{Li}_3 \left( \frac{1}{2} (1 - \sqrt{\eta}) \right) \\ &\quad - \frac{c_5}{\sqrt{2}} + \frac{1}{48(1-\eta)} \left[ 17\sqrt{2} - 17\eta\sqrt{2} + 2\frac{1}{\sqrt{\eta}} - 28\sqrt{\eta} + 14\eta^{3/2} \right] + \left[ \frac{1}{64\sqrt{\eta}} (18 \right. \\ &\quad - 6\eta + (2 - 15\sqrt{2})\sqrt{\eta}) - \frac{3 \ln(2)}{16} - \ln(\sqrt{2} - 1) + \ln(1 - \sqrt{\eta}) - \frac{17}{16} \ln(1 - \eta) \\ &\quad \left. + \frac{7 \ln(\eta)}{16} \right] \zeta_2 + \frac{7\zeta_3}{32\sqrt{\eta}} (2 - 3\sqrt{2}\sqrt{\eta} + 2\eta) + \left[ -\frac{5}{4\sqrt{2}} + \left( \frac{1}{8} (1 - 2i\pi) \right. \right. \\ &\quad \left. \left. + \frac{1}{4} \ln(1 - \eta) - \frac{\ln(\eta)}{4} \right) \ln(\sqrt{2} - 1) + \frac{1}{4} \ln^2(1 - \sqrt{\eta}) - \frac{1}{4} \ln(1 - \sqrt{\eta}) \ln(\eta) \right. \\ &\quad \left. + \frac{1}{4} \ln(1 - \eta) \ln(\eta) \right] \ln(2) + \left[ -\frac{1}{32} (1 + 2i\pi) + \frac{3}{16} \ln(\sqrt{2} - 1) - \frac{1}{4} \ln(1 - \sqrt{\eta}) \right. \\ &\quad \left. - \frac{1}{16} \ln(1 - \eta) - \frac{\ln(\eta)}{16} \right] \ln^2(2) - \frac{5}{12} \ln^3(2) - \frac{1}{4} i\pi \ln^2(\sqrt{2} - 1) + \frac{1}{12} \ln^3(\sqrt{2} - 1) \\ &\quad + \left[ -\frac{1}{4} i \ln(1 - \eta) (2\pi - i \ln(\eta)) + \frac{\ln(\eta)}{8} \right] \ln(1 - \sqrt{\eta}) - \frac{1}{12} \ln^3(1 - \sqrt{\eta}) \\ &\quad + \frac{1}{4} i\pi \ln^2(1 - \eta) - \frac{(3 - \eta)\sqrt{\eta} \ln(\eta)}{8(1 - \eta)^2} - \frac{1}{16} \ln(1 - \eta) \ln(\eta) + \left[ -\frac{1}{4} + \frac{\ln(2)}{2} \right. \\ &\quad \left. - \frac{1}{2} \ln(1 - \eta) + \frac{\ln(\eta)}{2} \right] \text{Li}_2 \left( \frac{1}{\sqrt{2}} \right) + \left[ -\frac{1}{2} \ln(1 - \eta) + \frac{\ln(\eta)}{2} \right] \text{Li}_2 \left( (\sqrt{2} - 1)^2 \right) \\ &\quad + \left[ \frac{1}{8} \ln(1 - \eta) - \frac{\ln(\eta)}{8} \right] \text{Li}_2 \left( (\sqrt{2} - 1)^4 \right) - \frac{1}{16} (1 + 2 \ln(\eta)) \text{Li}_2(\eta) + \text{Li}_3 \left( \frac{1}{\sqrt{2}} \right) \\ &\quad + \frac{1}{2} \text{Li}_3 \left( \frac{1}{2} \left( 1 - \frac{1}{\sqrt{2}} \right) \right) - \frac{1}{2} \text{Li}_3 \left( 1 - \frac{1}{\sqrt{2}} \right) - \frac{1}{2} \text{Li}_3 \left( 1 + \frac{1}{\sqrt{2}} \right) - \frac{1}{2} \text{Li}_3 \left( \frac{2}{1 - \sqrt{2}} \right) \\ &\quad + \frac{1}{2} \text{Li}_3(1 - \sqrt{\eta}) + \frac{1}{2} \text{Li}_3(1 + \sqrt{\eta}) - \frac{1}{8} \text{Li}_3(1 - \eta) - \text{Li}_3(\sqrt{\eta}) \\ &\quad \left. + \frac{1}{2} \text{Li}_3 \left( -\frac{2\sqrt{\eta}}{1 - \sqrt{\eta}} \right) + \frac{1}{8} \text{Li}_3(\eta) \right] \quad (\text{H.61}) \\ &= \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ -\frac{1}{12} \ln^3(1 - \sqrt{\eta}) - \frac{1}{4} \ln(\eta) \text{Li}_2 \left( \frac{1}{2} (1 + \sqrt{\eta}) \right) + \frac{1}{4} (1 + 2 \ln(\eta)) \text{Li}_2(\sqrt{\eta}) \right. \\ &\quad \left. + \frac{\text{Li}_3(1 - \sqrt{\eta})}{2} - \frac{1 - 14\eta + 7\eta^2}{24(-1 + \eta)} \frac{1}{\sqrt{\eta}} + \left[ -\frac{3}{32} (-3 + 4\sqrt{\eta} + \eta) \frac{1}{\sqrt{\eta}} + \frac{5 \ln(2)}{4} \right] \zeta_2 \right. \\ &\quad \left. + \frac{7}{16} (1 - \sqrt{\eta} + \eta) \frac{\zeta_3}{\sqrt{\eta}} + \left[ -\frac{1}{4} i \ln(1 - \eta) (2\pi - i \ln(\eta)) + \ln(\eta) \left( \frac{1}{8} - \frac{\ln(2)}{4} \right) - \frac{1}{4} \ln^2(2) \right] \right] \end{aligned}$$

$$\begin{aligned}
 & +\zeta_2 \left[ \ln(1-\sqrt{\eta}) + \left[ -\frac{3}{2}\zeta_2 + \ln(\eta) \left( -\frac{1}{16} + \frac{\ln(2)}{4} \right) \right] \ln(1-\eta) + \frac{1}{4}i\pi \ln(1-\eta)^2 \right. \\
 & + \left[ \frac{(-3+\eta)\sqrt{\eta}}{8(1-\eta)^2} + \frac{7}{8}\zeta_2 - \frac{1}{8}\ln^2(2) \right] \ln(\eta) + \ln(1-\sqrt{\eta})^2 \left( \frac{i\pi}{4} + \frac{3\ln(\eta)}{8} + \frac{\ln(2)}{4} \right) \\
 & + \frac{\ln^3(2)}{12} - \frac{1}{16}(1+2\ln(\eta))\text{Li}_2(\eta) - \frac{1}{2}\text{Li}_3\left(\frac{1}{2}(1-\sqrt{\eta})\right) + \frac{\text{Li}_3(1+\sqrt{\eta})}{2} - \frac{\text{Li}_3(1-\eta)}{8} \\
 & \left. - \text{Li}_3(\sqrt{\eta}) + \frac{1}{2}\text{Li}_3\left(\frac{2\sqrt{\eta}}{-1+\sqrt{\eta}}\right) + \frac{\text{Li}_3(\eta)}{8} \right] \tag{H.62}
 \end{aligned}$$

$$\begin{aligned}
 K_{22} & = G \left[ \left\{ \frac{\sqrt{(1-x)x}}{1-x(1-\eta)}, \frac{1}{x}, \sqrt{(1-x)x} \right\}, 1 \right] \\
 & = \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ -\frac{1}{8}i(2\pi - 3i\ln(\eta)) \ln^2(1-\sqrt{\eta}) + \frac{1}{4}\ln(2)\text{Li}_2\left(\frac{1}{2}(1+\frac{1}{\sqrt{2}})\right) \right. \\
 & + \frac{1}{4}\ln(\eta)\text{Li}_2\left(\frac{1}{2}(1+\sqrt{\eta})\right) + \frac{1}{2}\text{Li}_3\left(\frac{1}{2}(1-\sqrt{\eta})\right) - \frac{c_6}{\sqrt{2}} \\
 & + \frac{1}{48(1-\eta)} \left[ (1-\eta)\sqrt{2} - 14\frac{1}{\sqrt{\eta}} + 28\sqrt{\eta} - 2\eta^{3/2} \right] + \left[ \frac{1}{64\sqrt{\eta}}(6-18\eta \right. \\
 & - (2-3\sqrt{2})\sqrt{\eta}) + \frac{9\ln(2)}{16} + \ln(\sqrt{2}-1) - \ln(1-\sqrt{\eta}) + \frac{17}{16}\ln(1-\eta) \\
 & \left. - \frac{\ln(\eta)}{8} \right] \zeta_2 + \frac{7\zeta_3}{32\sqrt{\eta}} \left[ 2+2\eta - (1+3\sqrt{2})\sqrt{\eta} \right] + \left[ \frac{1}{4}\frac{1}{\sqrt{2}} - \frac{1}{4}\ln^2(1-\sqrt{\eta}) \right. \\
 & + \frac{1}{4}\ln(1-\sqrt{\eta})\ln(\eta) - \frac{1}{4}\ln(1-\eta)\ln(\eta) + \left( -\frac{1}{8} + \frac{i\pi}{4} - \frac{1}{4}\ln(1-\eta) \right) \ln(\sqrt{2}-1) \left. \right] \\
 & \times \ln(2) + \left[ \frac{1}{32}(1+2i\pi) - \frac{7}{16}\ln(\sqrt{2}-1) + \frac{1}{4}\ln(1-\sqrt{\eta}) + \frac{1}{16}\ln(1-\eta) + \frac{\ln(\eta)}{8} \right] \\
 & \times \ln^2(2) + \frac{1}{2}\ln^3(2) + \frac{1}{4}i\pi \ln^2(\sqrt{2}-1) - \frac{1}{12}\ln^3(\sqrt{2}-1) + \left[ \frac{1}{4}(2i\pi + \ln(\eta)) \ln(1-\eta) \right. \\
 & \left. - \frac{\ln(\eta)}{8} \right] \ln(1-\sqrt{\eta}) + \frac{1}{12}\ln^3(1-\sqrt{\eta}) - \frac{1}{4}i\pi \ln^2(1-\eta) - \frac{(1-3\eta)\sqrt{\eta}\ln(\eta)}{8(1-\eta)^2} \\
 & + \frac{1}{16}\ln(1-\eta)\ln(\eta) + \left[ \frac{1}{4} + \frac{\ln(2)}{2} + \frac{1}{2}\ln(1-\eta) \right] \text{Li}_2\left(\frac{1}{\sqrt{2}}\right) + \left[ \frac{\ln(2)}{2} \right. \\
 & + \frac{1}{2}\ln(1-\eta) \left. \right] \text{Li}_2\left((\sqrt{2}-1)^2\right) - \left[ \frac{\ln(2)}{8} + \frac{1}{8}\ln(1-\eta) \right] \text{Li}_2\left((\sqrt{2}-1)^4\right) \\
 & - \frac{1}{4}\text{Li}_2(\sqrt{\eta}) + \frac{1}{16}\text{Li}_2(\eta) + \text{Li}_3\left(\frac{1}{\sqrt{2}}\right) - \frac{1}{2}\text{Li}_3\left(\frac{1}{2}(1-\frac{1}{\sqrt{2}})\right) + \frac{1}{2}\text{Li}_3\left(1-\frac{1}{\sqrt{2}}\right) \\
 & + \frac{1}{2}\text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right) + \frac{1}{2}\text{Li}_3\left(-\frac{2}{-1+\sqrt{2}}\right) - \frac{1}{2}\text{Li}_3(1-\sqrt{\eta}) - \frac{1}{2}\text{Li}_3(1+\sqrt{\eta}) \\
 & \left. + \frac{1}{8}\text{Li}_3(1-\eta) - \text{Li}_3(\sqrt{\eta}) - \frac{1}{2}\text{Li}_3\left(-\frac{2\sqrt{\eta}}{1-\sqrt{\eta}}\right) + \frac{1}{8}\text{Li}_3(\eta) \right] \tag{H.63} \\
 & = \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ \frac{1}{12}\ln^3(1-\sqrt{\eta}) + \frac{1}{4}\ln(\eta)\text{Li}_2\left(\frac{1}{2}(1+\sqrt{\eta})\right) - \frac{\text{Li}_3(1-\sqrt{\eta})}{2} - \frac{7-14\eta+\eta^2}{24(1-\eta)\sqrt{\eta}} \right.
 \end{aligned}$$

$$\begin{aligned}
 & + \left[ -\frac{3}{32}(-1 - 4\sqrt{\eta} + 3\eta) \frac{1}{\sqrt{\eta}} - \frac{5 \ln(2)}{4} \right] \zeta_2 + \frac{7}{16}(1 + \sqrt{\eta} + \eta) \frac{\zeta_3}{\sqrt{\eta}} - \frac{1}{12} \ln^3(2) \\
 & + \left[ \frac{1}{4} \ln(1 - \eta)(2i\pi + \ln(\eta)) - \zeta_2 + \frac{\ln(2)^2}{4} + \frac{1}{8}(-1 + 2 \ln(2)) \ln(\eta) \right] \ln(1 - \sqrt{\eta}) \\
 & + \left[ -\frac{i\pi}{4} - \frac{\ln(2)}{4} - \frac{3 \ln(\eta)}{8} \right] \ln(1 - \sqrt{\eta})^2 + \left[ \frac{3}{2} \zeta_2 + \frac{1}{16}(1 - 4 \ln(2)) \ln(\eta) \right] \ln(1 - \eta) \\
 & - \frac{1}{4} i\pi \ln^2(1 - \eta) + \left[ \frac{(-1 + 3\eta)\sqrt{\eta}}{8(1 - \eta)^2} - \frac{1}{8} \zeta_2 + \frac{\ln(2)^2}{8} \right] \ln(\eta) - \frac{\text{Li}_2(\sqrt{\eta})}{4} + \frac{\text{Li}_2(\eta)}{16} \\
 & + \frac{1}{2} \text{Li}_3\left(\frac{1}{2}(1 - \sqrt{\eta})\right) - \frac{1}{2} \text{Li}_3(1 + \sqrt{\eta}) + \frac{\text{Li}_3(1 - \eta)}{8} - \text{Li}_3(\sqrt{\eta}) - \frac{1}{2} \text{Li}_3\left(\frac{2\sqrt{\eta}}{-1 + \sqrt{\eta}}\right) \\
 & + \frac{\text{Li}_3(\eta)}{8} \tag{H.64}
 \end{aligned}$$

$$\begin{aligned}
 K_{23} & = G \left[ \left\{ \frac{\sqrt{(1-x)x}}{1-x(1-\eta)}, \sqrt{(1-x)x}, \frac{1}{1-x} \right\}, 1 \right] \\
 & = \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ \frac{1}{4}(1 - 2 \ln(2)) \text{Li}_2\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{4} \ln(2) \text{Li}_2\left(\frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right)\right) \right. \\
 & + \frac{1}{4} \ln(\eta) \text{Li}_2\left(\frac{1}{2}(1 + \sqrt{\eta})\right) - \frac{1}{4}(1 + 2 \ln(\eta)) \text{Li}_2(\sqrt{\eta}) - \frac{1}{2} \text{Li}_3\left(\frac{\sqrt{\eta}}{1 + \sqrt{\eta}}\right) - \frac{c_7}{\sqrt{2}} \\
 & - \frac{1}{288(1-\eta)\sqrt{\eta}}(-94 - 136\eta + 14\eta^2 + 317\sqrt{2}\sqrt{\eta} - 317\sqrt{2}\eta^{3/2}) \\
 & + \left. \left[ \frac{\ln(2)}{16\sqrt{\eta}}(6 + 6\eta - 3(1 + 3\sqrt{2})\sqrt{\eta}) + \frac{1}{64(1-\eta)^2\sqrt{\eta}}(-6 - 10\eta - 10\eta^2 \right. \right. \\
 & - 6\eta^3 + (-2 + 33\sqrt{2})\sqrt{\eta} + (4 - 66\sqrt{2})\eta^{3/2} + (-2 + 33\sqrt{2})\eta^{5/2}) - \frac{\ln(\eta)}{8} \left. \right] \zeta_2 \\
 & - \frac{7\zeta_3}{64\sqrt{\eta}} \left[ 2 + 2\eta - (2 + 3\sqrt{2})\sqrt{\eta} \right] + \left[ \left(-\frac{1}{8} - \frac{i\pi}{4}\right) \ln(\sqrt{2} - 1) + \frac{5}{4\sqrt{2}} \right. \\
 & - \frac{1}{4} \ln^2(\sqrt{2} - 1) + \left(-\frac{1}{2} \ln(1 - \eta) + \frac{\ln(\eta)}{4}\right) \ln(1 - \sqrt{\eta}) + \frac{1}{4} \ln^2(1 - \sqrt{\eta}) \\
 & + \frac{1}{4} \ln^2(1 - \eta) - \frac{1}{4} \ln(1 - \eta) \ln(\eta) \left. \right] \ln(2) + \left( \frac{1}{32}(1 - 2i\pi) - \frac{1}{8} \ln(\sqrt{2} - 1) \right. \\
 & + \frac{1}{4} \ln(1 - \sqrt{\eta}) - \frac{1}{4} \ln(1 - \eta) + \frac{\ln(\eta)}{8} \left. \right) \ln^2(2) + \frac{\ln^3(2)}{24} - \frac{1}{4} i\pi \ln^2(\sqrt{2} - 1) \\
 & + \left[ -\frac{1}{2} i\pi \ln(1 - \eta) - \frac{\ln(\eta)}{8} - \frac{1}{8} \ln^2(\eta) \right] \ln(1 - \sqrt{\eta}) + \frac{1}{4} i\pi \ln^2(1 - \sqrt{\eta}) \\
 & + \left[ \frac{\ln(\eta)}{16(1-\eta)^2}(1 - 2\eta + \eta^2 + 4\sqrt{\eta} + 4\eta^{3/2}) + \frac{\ln(\eta)^2}{16} \right] \ln(1 - \eta) + \frac{1}{4} i\pi \ln^2(1 - \eta) \\
 & - \frac{(-3 + \eta)\sqrt{\eta} \ln(\eta)}{8(1-\eta)^2} - \frac{(1 + \eta)\sqrt{\eta} \ln^2(\eta)}{8(1-\eta)^2} + \left[ \frac{1}{16(1-\eta)^2}(1 - 2\eta + \eta^2 + 4\sqrt{\eta} \right. \\
 & + 4\eta^{3/2}) + \frac{\ln(\eta)}{8} \left. \right] \text{Li}_2(\eta) - \frac{1}{2} \text{Li}_3\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{2} \text{Li}_3\left(\frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right)\right) - \frac{1}{2} \text{Li}_3\left(1 + \frac{1}{\sqrt{2}}\right)
 \end{aligned}$$



$$\begin{aligned}
 & + \frac{1}{2} \text{Li}_3 \left( \frac{1}{1 + \sqrt{2}} \right) - \frac{1}{2} \text{Li}_3 \left( \frac{2}{1 + \sqrt{2}} \right) - \frac{1}{2} \text{Li}_3 \left( \frac{1}{2} (1 + \sqrt{\eta}) \right) + \frac{1}{2} \text{Li}_3 (1 + \sqrt{\eta}) \\
 & - \frac{1}{8} \text{Li}_3 (1 - \eta) + \frac{1}{2} \text{Li}_3 (\sqrt{\eta}) + \frac{1}{2} \text{Li}_3 \left( \frac{2\sqrt{\eta}}{1 + \sqrt{\eta}} \right) - \frac{1}{8} \text{Li}_3 (\eta) \Big] \tag{H.65}
 \end{aligned}$$

$$\begin{aligned}
 = & \frac{\sqrt{\eta}}{(1 - \eta)^2} \left[ \frac{1}{12} \ln^3 (1 - \sqrt{\eta}) + \frac{1}{4} \ln(\eta) \text{Li}_2 \left( \frac{1}{2} (1 + \sqrt{\eta}) \right) - \frac{1}{4} (1 + 2 \ln(\eta)) \text{Li}_2 (\sqrt{\eta}) \right. \\
 & + \frac{47 + 68\eta - 7\eta^2}{144(1 - \eta)\sqrt{\eta}} + \left. \left[ \frac{\ln(2)}{8} \left( -10 + 3 \frac{1}{\sqrt{\eta}} + 3\sqrt{\eta} \right) - \frac{1}{32(1 - \eta)^2\sqrt{\eta}} (3 + 5\eta + 5\eta^2 \right. \right. \\
 & + \left. \left. 3\eta^3 - 12\sqrt{\eta} + 24\eta^{3/2} - 12\eta^{5/2}) \right] \zeta_2 - \frac{7}{32} (-1 + \sqrt{\eta})^2 \frac{\zeta_3}{\sqrt{\eta}} - \frac{1}{12} \ln(2)^3 + \left[ \frac{1}{2} \zeta_2 \right. \right. \\
 & + \left. \frac{\ln^2(2)}{4} + \left( -\frac{1}{8} + \frac{\ln(2)}{4} + \frac{1}{4} \ln(1 - \eta) \right) \ln(\eta) - \frac{1}{8} \ln^2(\eta) \right] \ln(1 - \sqrt{\eta}) - \left[ \frac{\ln(2)}{4} \right. \\
 & + \left. \frac{3 \ln(\eta)}{8} \right] \ln^2(1 - \sqrt{\eta}) + \left[ -\frac{(-3 + \eta)\sqrt{\eta}}{8(1 - \eta)^2} - \frac{1}{8} \zeta_2 + \frac{\ln^2(2)}{8} + \left( \frac{1}{16(1 - \eta)^2} (1 - 2\eta \right. \right. \\
 & + \left. \left. \eta^2 + 4\sqrt{\eta} + 4\eta^{3/2}) - \frac{\ln(2)}{4} \right) \ln(1 - \eta) \right] \ln(\eta) + \left[ -\frac{(1 + \eta)\sqrt{\eta}}{8(1 - \eta)^2} + \frac{1}{16} \ln(1 - \eta) \right] \ln^2(\eta) \\
 & + \left[ \frac{1}{16(1 - \eta)^2} (1 - 2\eta + \eta^2 + 4\sqrt{\eta} + 4\eta^{3/2}) + \frac{\ln(\eta)}{8} \right] \text{Li}_2(\eta) + \frac{1}{2} \text{Li}_3 \left( \frac{1}{2} (1 - \sqrt{\eta}) \right) \\
 & - \text{Li}_3 (1 - \sqrt{\eta}) + \frac{\text{Li}_3(1 - \eta)}{8} - \frac{1}{2} \text{Li}_3 \left( \frac{2\sqrt{\eta}}{-1 + \sqrt{\eta}} \right) \Big] \tag{H.66}
 \end{aligned}$$

$$\begin{aligned}
 K_{24} & = G \left[ \left\{ \frac{\sqrt{x(1-x)}}{1-x(1-\eta)}, \sqrt{x(1-x)}, \frac{1}{x} \right\}, 1 \right] \\
 & = \frac{\sqrt{\eta}}{(1 - \eta)^2} \left[ -\frac{1}{4} \ln(2) \text{Li}_2 \left( \frac{1}{2} \left( 1 + \frac{1}{\sqrt{2}} \right) \right) - \frac{1}{4} \ln(\eta) \text{Li}_2 \left( \frac{1}{2} (1 + \sqrt{\eta}) \right) \right. \\
 & + \frac{1}{2} \text{Li}_3 \left( \frac{\sqrt{\eta}}{1 + \sqrt{\eta}} \right) - \frac{\ln(1 - \eta) \ln(\eta)}{16(1 - \eta)^2} (1 - 2\eta + \eta^2 + 4\sqrt{\eta} + 4\eta^{3/2}) \\
 & - \frac{1}{16(1 - \eta)^2} \text{Li}_2(\eta) (1 - 2\eta + \eta^2 + 4\sqrt{\eta} + 4\eta^{3/2}) - \frac{c_8}{\sqrt{2}} \\
 & - \frac{1}{288(-1 + \eta)} \left( 155\sqrt{2}(1 - \eta) + 14 \frac{1}{\sqrt{\eta}} - 136\sqrt{\eta} - 94\eta^{3/2} \right) + \left[ \frac{\ln(2)}{16\sqrt{\eta}} (-6(1 + \eta) \right. \\
 & + \left. (3 + 9\sqrt{2})\sqrt{\eta}) + \frac{1}{64(1 - \eta)^2\sqrt{\eta}} (6 + 10\eta + 10\eta^2 + 6\eta^3 + (2 - 33\sqrt{2})\sqrt{\eta} \right. \\
 & + \left. (-4 + 66\sqrt{2})\eta^{3/2} + (2 - 33\sqrt{2})\eta^{5/2}) + \frac{\ln(\eta)}{8} \right] \zeta_2 - \frac{7\zeta_3}{64\sqrt{\eta}} \left[ 2 + 2\eta + (1 - 3\sqrt{2})\sqrt{\eta} \right] \\
 & + \left[ \frac{1}{8} (1 + 2i\pi) \ln(\sqrt{2} - 1) - \frac{1}{4\sqrt{2}} + \frac{1}{4} \ln^2(\sqrt{2} - 1) + \left( \frac{1}{2} \ln(1 - \eta) \right. \right. \\
 & - \left. \left. \frac{\ln(\eta)}{4} \right) \ln(1 - \sqrt{\eta}) - \frac{1}{4} \ln^2(1 - \sqrt{\eta}) - \frac{1}{4} \ln^2(1 - \eta) + \frac{1}{4} \ln(1 - \eta) \ln(\eta) \right] \ln(2) \\
 & + \left[ \frac{1}{32} (-1 + 12\sqrt{2} + 2i\pi) + \frac{1}{4} \ln(\sqrt{2} - 1) - \frac{1}{4} \ln(1 - \sqrt{\eta}) + \frac{1}{4} \ln(1 - \eta) \right.
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{\ln(\eta)}{8} \Big] \ln^2(2) - \frac{1}{12} \ln(2)^3 + \frac{1}{4} i\pi \ln^2(\sqrt{2}-1) + \left[ \frac{1}{2} i\pi \ln(1-\eta) + \frac{\ln(\eta)}{8} \right] \ln(1-\sqrt{\eta}) \\
 & -\frac{1}{4} i\pi \ln^2(1-\sqrt{\eta}) - \frac{1}{4} i\pi \ln^2(1-\eta) + \frac{(1-3\eta)\sqrt{\eta}\ln(\eta)}{8(1-\eta)^2} - \frac{1}{4} \text{Li}_2\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{4} \text{Li}_2(\sqrt{\eta}) \\
 & -\frac{1}{2} \text{Li}_3\left(\frac{1}{\sqrt{2}}\right) - \frac{1}{2} \text{Li}_3\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) + \frac{1}{2} \text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right) - \frac{1}{2} \text{Li}_3\left(\frac{1}{1+\sqrt{2}}\right) \\
 & +\frac{1}{2} \text{Li}_3\left(\frac{2}{1+\sqrt{2}}\right) + \frac{1}{2} \text{Li}_3\left(\frac{1}{2}(1+\sqrt{\eta})\right) - \frac{1}{2} \text{Li}_3(1+\sqrt{\eta}) + \frac{1}{8} \text{Li}_3(1-\eta) \\
 & +\frac{1}{2} \text{Li}_3(\sqrt{\eta}) - \frac{1}{2} \text{Li}_3\left(\frac{2\sqrt{\eta}}{1+\sqrt{\eta}}\right) \Big] \tag{H.67}
 \end{aligned}$$

$$\begin{aligned}
 = & \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ -\frac{1}{12} \ln^3(1-\sqrt{\eta}) + \frac{1}{8} \ln^2(1-\sqrt{\eta})(3\ln(\eta) + 2\ln(2)) - \frac{\text{Li}_2(\eta)}{16(1-\eta)^2} (1-2\eta \right. \\
 & +\eta^2 + 4\sqrt{\eta} + 4\eta^{3/2}) - \frac{1}{4} \ln(\eta) \text{Li}_2\left(\frac{1}{2}(1+\sqrt{\eta})\right) + \frac{7-68\eta-47\eta^2}{144(1-\eta)\sqrt{\eta}} + \left. \left[ \frac{1}{32(1-\eta)^2} \right. \right. \\
 & \times (3+5\eta+5\eta^2+3\eta^3-12\sqrt{\eta}+24\eta^{3/2}-12\eta^{5/2}) \frac{1}{\sqrt{\eta}} + \frac{1}{8} (10-3\frac{1}{\sqrt{\eta}}-3\sqrt{\eta}) \ln(2) \Big] \zeta_2 \\
 & -\frac{7}{32} (1+\sqrt{\eta})^2 \frac{\zeta_3}{\sqrt{\eta}} - \left. \left[ \frac{1}{2} \zeta_2 - \ln(\eta) \left( \frac{1}{8} - \frac{1}{4} \ln(1-\eta) - \frac{\ln(2)}{4} \right) + \frac{1}{4} \ln^2(2) \right] \ln(1-\sqrt{\eta}) \right. \\
 & + \left. \left[ -\frac{(-1+3\eta)\sqrt{\eta}}{8(1-\eta)^2} + \frac{1}{8} \zeta_2 - \left( \frac{1}{16(1-\eta)^2} (1-2\eta+\eta^2+4\sqrt{\eta}+4\eta^{3/2}) - \frac{\ln(2)}{4} \right) \right. \right. \\
 & \times \ln(1-\eta) - \frac{1}{8} \ln^2(2) \Big] \ln(\eta) + \frac{\ln^3(2)}{12} + \frac{\text{Li}_2(\sqrt{\eta})}{4} - \frac{1}{2} \text{Li}_3\left(\frac{1}{2}(1-\sqrt{\eta})\right) \\
 & \left. +\text{Li}_3(1-\sqrt{\eta}) - \frac{\text{Li}_3(1-\eta)}{8} + \text{Li}_3(\sqrt{\eta}) + \frac{1}{2} \text{Li}_3\left(\frac{2\sqrt{\eta}}{-1+\sqrt{\eta}}\right) - \frac{\text{Li}_3(\eta)}{8} \right] \tag{H.68}
 \end{aligned}$$

$$\begin{aligned}
 K_{25} & = G \left[ \left\{ -\frac{\sqrt{x(1-x)}}{\eta+x(1-\eta)}, \frac{1}{1-x}, \sqrt{x(1-x)} \right\}, 1 \right] \\
 & = \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ \frac{1}{8} (2i\pi + 3\ln(\eta)) \ln^2(1-\sqrt{\eta}) - \frac{1}{4} \ln(2) \text{Li}_2\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) \right. \\
 & -\frac{1}{4} \ln(\eta) \text{Li}_2\left(\frac{1}{2}(1+\sqrt{\eta})\right) - \frac{1}{2} \text{Li}_3\left(\frac{1}{2}(1-\sqrt{\eta})\right) - \frac{1}{48(1-\eta)} \left( \sqrt{2}(1-\eta) - 14\frac{1}{\sqrt{\eta}} \right. \\
 & +28\sqrt{\eta} - 2\eta^{3/2} ) - \frac{c_2}{\sqrt{2}} + \left. \left[ \frac{1}{64\sqrt{\eta}} (6-18\eta+(2+3\sqrt{2})\sqrt{\eta}) + \frac{3\ln(2)}{16} \right. \right. \\
 & +\frac{1}{2} \ln(\sqrt{2}-1) - \frac{1}{2} \ln(1-\sqrt{\eta}) + \frac{7}{16} \ln(1-\eta) + \frac{\ln(\eta)}{8} \Big] \zeta_2 - \frac{7\zeta_3}{32\sqrt{\eta}} \left[ 2(1+\eta) \right. \\
 & - (1+3\sqrt{2})\sqrt{\eta} \Big] + \left. \left[ -\frac{1}{4\sqrt{2}} + \left( \frac{1}{8}(1-2i\pi) + \frac{1}{4} \ln(1-\eta) \right) \ln(\sqrt{2}-1) \right. \right. \\
 & +\frac{1}{4} \ln^2(1-\sqrt{\eta}) - \frac{1}{4} \ln(1-\sqrt{\eta}) \ln(\eta) + \frac{1}{4} \ln(1-\eta) \ln(\eta) \Big] \ln(2) + \left. \left[ -\frac{1}{32}(1+2i\pi) \right. \right. \\
 & \left. \left. +\frac{7}{16} \ln(\sqrt{2}-1) - \frac{1}{4} \ln(1-\sqrt{\eta}) - \frac{1}{16} \ln(1-\eta) - \frac{\ln(\eta)}{8} \right] \ln^2(2) - \frac{1}{2} \ln^3(2) \right]
 \end{aligned}$$

$$\begin{aligned}
 & -\frac{1}{4}i\pi \ln^2(\sqrt{2}-1) + \frac{1}{12} \ln^3(\sqrt{2}-1) + \left[ -\frac{1}{4}i \ln(1-\eta)(2\pi - i \ln(\eta)) \right. \\
 & \left. + \frac{\ln(\eta)}{8} \right] \ln(1-\sqrt{\eta}) - \frac{1}{12} \ln^3(1-\sqrt{\eta}) + \frac{1}{4}i\pi \ln^2(1-\eta) + \frac{(1-3\eta)\sqrt{\eta} \ln(\eta)}{8(1-\eta)^2} \\
 & - \frac{1}{16} \ln(1-\eta) \ln(\eta) + \left[ -\frac{1}{4} - \frac{\ln(2)}{2} - \frac{1}{2} \ln(1-\eta) \right] \text{Li}_2\left(\frac{1}{\sqrt{2}}\right) + \left[ -\frac{\ln(2)}{2} \right. \\
 & \left. - \frac{1}{2} \ln(1-\eta) \right] \text{Li}_2\left((\sqrt{2}-1)^2\right) + \left[ \frac{\ln(2)}{8} + \frac{1}{8} \ln(1-\eta) \right] \text{Li}_2\left((\sqrt{2}-1)^4\right) + \frac{1}{4} \text{Li}_2(\sqrt{\eta}) \\
 & - \frac{1}{16} \text{Li}_2(\eta) - \text{Li}_3\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{2} \text{Li}_3\left(\frac{1}{2}\left(1-\frac{1}{\sqrt{2}}\right)\right) - \frac{1}{2} \text{Li}_3\left(1-\frac{1}{\sqrt{2}}\right) - \frac{1}{2} \text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right) \\
 & - \frac{1}{2} \text{Li}_3\left(-\frac{2}{-1+\sqrt{2}}\right) + \frac{1}{2} \text{Li}_3(1-\sqrt{\eta}) + \frac{1}{2} \text{Li}_3(1+\sqrt{\eta}) - \frac{1}{8} \text{Li}_3(1-\eta) + \text{Li}_3(\sqrt{\eta}) \\
 & \left. + \frac{1}{2} \text{Li}_3\left(-\frac{2\sqrt{\eta}}{1-\sqrt{\eta}}\right) - \frac{1}{8} \text{Li}_3(\eta) \right] \tag{H.69}
 \end{aligned}$$

$$\begin{aligned}
 = & \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ -\frac{1}{12} \ln^3(1-\sqrt{\eta}) - \frac{1}{16} (1-4\ln(2)) \ln(1-\eta) \ln(\eta) - \frac{1}{4} \ln(\eta) \text{Li}_2\left(\frac{(1+\sqrt{\eta})}{2}\right) \right. \\
 & \left. + \frac{\text{Li}_3(1-\sqrt{\eta})}{2} + \frac{7-14\eta+\eta^2}{24(1-\eta)\sqrt{\eta}} + \left[ \frac{3}{32} (1-3\eta) \frac{1}{\sqrt{\eta}} - \frac{\ln(2)}{4} \right] \zeta_2 - \frac{7}{16} (1+\sqrt{\eta}+\eta) \frac{\zeta_3}{\sqrt{\eta}} \right. \\
 & \left. + \frac{\ln^3(2)}{12} + \left[ -\frac{1}{4} i \ln(1-\eta)(2\pi - i \ln(\eta)) - \frac{1}{2} \zeta_2 - \frac{1}{4} \ln^2(2) + \frac{1}{8} (1-2\ln(2)) \ln(\eta) \right] \right. \\
 & \times \ln(1-\sqrt{\eta}) + \left[ \frac{i\pi}{4} + \frac{\ln(2)}{4} + \frac{3\ln(\eta)}{8} \right] \ln^2(1-\sqrt{\eta}) + \frac{1}{4} i\pi \ln^2(1-\eta) \\
 & \left. + \left( \frac{(1-3\eta)\sqrt{\eta}}{8(1-\eta)^2} + \frac{1}{8} \zeta_2 - \frac{1}{8} \ln^2(2) \right) \ln(\eta) + \frac{\text{Li}_2(\sqrt{\eta})}{4} - \frac{\text{Li}_2(\eta)}{16} - \frac{1}{2} \text{Li}_3\left(\frac{1}{2}(1-\sqrt{\eta})\right) \right. \\
 & \left. + \frac{\text{Li}_3(1+\sqrt{\eta})}{2} - \frac{\text{Li}_3(1-\eta)}{8} + \text{Li}_3(\sqrt{\eta}) + \frac{1}{2} \text{Li}_3\left(\frac{2\sqrt{\eta}}{-1+\sqrt{\eta}}\right) - \frac{\text{Li}_3(\eta)}{8} \right] \tag{H.70}
 \end{aligned}$$

$$\begin{aligned}
 K_{26} & = G \left[ \left\{ -\frac{\sqrt{(1-x)x}}{\eta+x(1-\eta)}, \frac{1}{x}, \sqrt{(1-x)x} \right\}, 1 \right] \\
 & = \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ -\frac{1}{8} i (2\pi - 3i \ln(\eta)) \ln^2(1-\sqrt{\eta}) + \frac{1}{4} \ln(2) \text{Li}_2\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) \right. \\
 & \left. + \frac{1}{4} \ln(\eta) \text{Li}_2\left(\frac{1}{2}(1+\sqrt{\eta})\right) - \frac{1}{4} (1+2\ln(\eta)) \text{Li}_2(\sqrt{\eta}) + \frac{1}{2} \text{Li}_3\left(\frac{1}{2}(1-\sqrt{\eta})\right) \right. \\
 & \left. - \frac{1}{48(1-\eta)} \left( 17\sqrt{2}(1-\eta) + 2\frac{1}{\sqrt{\eta}} - 28\sqrt{\eta} + 14\eta^{3/2} \right) - \frac{c_1}{\sqrt{2}} + \left[ \frac{1}{64\sqrt{\eta}} (18-6\eta \right. \right. \\
 & \left. \left. - (2+15\sqrt{2})\sqrt{\eta} \right) + \frac{3\ln(2)}{16} - \frac{1}{2} \ln(\sqrt{2}-1) + \frac{1}{2} \ln(1-\sqrt{\eta}) - \frac{7}{16} \ln(1-\eta) \right. \\
 & \left. + \frac{5\ln(\eta)}{16} \right] \zeta_2 - \frac{7\zeta_3}{32\sqrt{\eta}} \left[ 2-3\sqrt{2}\sqrt{\eta}+2\eta \right] + \left[ \frac{5}{4\sqrt{2}} + \left( -\frac{1}{8} + \frac{i\pi}{4} - \frac{1}{4} \ln(1-\eta) \right) \right. \\
 & \left. + \frac{\ln(\eta)}{4} \right] \ln(\sqrt{2}-1) - \frac{1}{4} \ln^2(1-\sqrt{\eta}) + \frac{1}{4} \ln(1-\sqrt{\eta}) \ln(\eta) - \frac{1}{4} \ln(1-\eta) \ln(\eta) \left. \right] \ln(2)
 \end{aligned}$$

$$\begin{aligned}
 & + \left( \frac{1}{32}(1 + 2i\pi) - \frac{3}{16} \ln(\sqrt{2} - 1) + \frac{1}{4} \ln(1 - \sqrt{\eta}) + \frac{1}{16} \ln(1 - \eta) + \frac{\ln(\eta)}{16} \right) \ln^2(2) \\
 & + \frac{5 \ln^3(2)}{12} + \frac{1}{4} i\pi \ln^2(\sqrt{2} - 1) - \frac{1}{12} \ln^3(\sqrt{2} - 1) + \left( \frac{1}{4} (2i\pi + \ln(\eta)) \ln(1 - \eta) \right. \\
 & \left. - \frac{\ln(\eta)}{8} \right) \ln(1 - \sqrt{\eta}) + \frac{1}{12} \ln^3(1 - \sqrt{\eta}) - \frac{1}{4} i\pi \ln^2(1 - \eta) + \frac{(3 - \eta)\sqrt{\eta} \ln(\eta)}{8(1 - \eta)^2} \\
 & + \frac{1}{16} \ln(1 - \eta) \ln(\eta) + \left[ \frac{1}{4} - \frac{\ln(2)}{2} + \frac{1}{2} \ln(1 - \eta) - \frac{\ln(\eta)}{2} \right] \text{Li}_2 \left( \frac{1}{\sqrt{2}} \right) \\
 & + \left[ \frac{1}{2} \ln(1 - \eta) - \frac{\ln(\eta)}{2} \right] \text{Li}_2 \left( (\sqrt{2} - 1)^2 \right) + \left[ -\frac{1}{8} \ln(1 - \eta) + \frac{\ln(\eta)}{8} \right] \text{Li}_2 \left( (\sqrt{2} - 1)^4 \right) \\
 & + \frac{1}{16} (1 + 2 \ln(\eta)) \text{Li}_2(\eta) - \text{Li}_3 \left( \frac{1}{\sqrt{2}} \right) - \frac{1}{2} \text{Li}_3 \left( \frac{1}{2} \left( 1 - \frac{1}{\sqrt{2}} \right) \right) + \frac{1}{2} \text{Li}_3 \left( 1 - \frac{1}{\sqrt{2}} \right) \\
 & + \frac{1}{2} \text{Li}_3 \left( 1 + \frac{1}{\sqrt{2}} \right) + \frac{1}{2} \text{Li}_3 \left( -\frac{2}{-1 + \sqrt{2}} \right) - \frac{1}{2} \text{Li}_3(1 - \sqrt{\eta}) - \frac{1}{2} \text{Li}_3(1 + \sqrt{\eta}) \\
 & + \frac{1}{8} \text{Li}_3(1 - \eta) + \text{Li}_3(\sqrt{\eta}) - \frac{1}{2} \text{Li}_3 \left( -\frac{2\sqrt{\eta}}{1 - \sqrt{\eta}} \right) - \frac{1}{8} \text{Li}_3(\eta) \Big] \tag{H.71}
 \end{aligned}$$

$$\begin{aligned}
 = & \frac{\sqrt{\eta}}{(1 - \eta)^2} \left[ \frac{1}{12} \ln^3(1 - \sqrt{\eta}) + \frac{1}{16} (1 - 4 \ln(2)) \ln(1 - \eta) \ln(\eta) + \frac{1}{4} \ln(\eta) \text{Li}_2 \left( \frac{1}{2} (1 + \sqrt{\eta}) \right) \right. \\
 & \left. - \frac{1}{4} (1 + 2 \ln(\eta)) \text{Li}_2(\sqrt{\eta}) - \frac{\text{Li}_3(1 - \sqrt{\eta})}{2} + \frac{1 - 14\eta + 7\eta^2}{24(-1 + \eta)} \frac{1}{\sqrt{\eta}} + \left[ \frac{3}{32} (3 - \eta) \frac{1}{\sqrt{\eta}} \right. \right. \\
 & \left. \left. + \frac{\ln(2)}{4} \right] \zeta_2 - \frac{7}{16} (1 - \sqrt{\eta} + \eta) \frac{\zeta_3}{\sqrt{\eta}} - \frac{1}{12} \ln^3(2) + \left[ \frac{1}{4} \ln(1 - \eta) (2i\pi + \ln(\eta)) + \frac{1}{2} \zeta_2 \right. \right. \\
 & \left. \left. + \frac{\ln^2(2)}{4} - \frac{1}{8} (1 - 2 \ln(2)) \ln(\eta) \right] \ln(1 - \sqrt{\eta}) - \left[ \frac{i\pi}{4} + \frac{\ln(2)}{4} + \frac{3 \ln(\eta)}{8} \right] \ln^2(1 - \sqrt{\eta}) \right. \\
 & \left. - \frac{1}{4} i\pi \ln(1 - \eta)^2 + \left[ \frac{(3 - \eta)\sqrt{\eta}}{8(1 - \eta)^2} - \frac{1}{8} \zeta_2 + \frac{\ln^2(2)}{8} \right] \ln(\eta) + \frac{1}{16} (1 + 2 \ln(\eta)) \text{Li}_2(\eta) \right. \\
 & \left. + \frac{1}{2} \text{Li}_3 \left( \frac{1}{2} (1 - \sqrt{\eta}) \right) - \frac{1}{2} \text{Li}_3(1 + \sqrt{\eta}) + \frac{\text{Li}_3(1 - \eta)}{8} + \text{Li}_3(\sqrt{\eta}) \right. \\
 & \left. - \frac{1}{2} \text{Li}_3 \left( \frac{2\sqrt{\eta}}{-1 + \sqrt{\eta}} \right) - \frac{\text{Li}_3(\eta)}{8} \right] \tag{H.72}
 \end{aligned}$$

$$\begin{aligned}
 K_{27} & = G \left[ \left\{ -\frac{\sqrt{(1-x)x}}{\eta + x(1-\eta)}, \sqrt{(1-x)x}, \frac{1}{1-x} \right\}, 1 \right] \\
 & = \frac{\sqrt{\eta}}{(1 - \eta)^2} \left[ \frac{1}{4} \ln(2) \text{Li}_2 \left( \frac{1}{2} \left( 1 + \frac{1}{\sqrt{2}} \right) \right) + \frac{1}{4} \ln(\eta) \text{Li}_2 \left( \frac{1}{2} (1 + \sqrt{\eta}) \right) \right. \\
 & \left. - \frac{1}{2} \text{Li}_3 \left( \frac{\sqrt{\eta}}{1 + \sqrt{\eta}} \right) + \frac{\ln(1 - \eta) \ln(\eta)}{16(1 - \eta)^2} \left( 1 - 2\eta + \eta^2 + 4\sqrt{\eta} + 4\eta^{3/2} \right) \right. \\
 & \left. + \frac{1}{16(1 - \eta)^2} \text{Li}_2(\eta) \left( 1 - 2\eta + \eta^2 + 4\sqrt{\eta} + 4\eta^{3/2} \right) - \frac{c_4}{\sqrt{2}} - \frac{1}{288(1 - \eta)\sqrt{\eta}} \left( 14 \right. \right. \\
 & \left. \left. - 136\eta - 94\eta^2 + 155\sqrt{2}\sqrt{\eta} - 155\sqrt{2}\eta^{3/2} \right) + \left[ -\frac{3 \ln(2)}{16\sqrt{\eta}} \left( 2(1 + \eta) + (1 - 3\sqrt{2})\sqrt{\eta} \right) \right. \right.
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{64(1-\eta)^2\sqrt{\eta}} \left( 6 - 22\eta - 22\eta^2 + 6\eta^3 + (-2 + 15\sqrt{2})\sqrt{\eta} + (4 - 30\sqrt{2})\eta^{3/2} \right. \\
 & \left. + (-2 + 15\sqrt{2})\eta^{5/2} \right) - \frac{\ln(\eta)}{8} \Big] \zeta_2 + \frac{7\zeta_3}{64\sqrt{\eta}} \left[ 2 + 2\eta + (1 - 3\sqrt{2})\sqrt{\eta} \right] \\
 & + \left[ \left( -\frac{1}{8} - \frac{i\pi}{4} \right) \ln(\sqrt{2} - 1) + \frac{1}{4\sqrt{2}} - \frac{1}{4} \ln^2(\sqrt{2} - 1) + \left( -\frac{1}{2} \ln(1 - \eta) \right. \right. \\
 & \left. \left. + \frac{\ln(\eta)}{4} \right) \ln(1 - \sqrt{\eta}) + \frac{1}{4} \ln^2(1 - \sqrt{\eta}) + \frac{1}{4} \ln^2(1 - \eta) - \frac{1}{4} \ln(1 - \eta) \ln(\eta) \right] \ln(2) \\
 & + \left[ \frac{1}{32} (1 - 12\sqrt{2} - 2i\pi) - \frac{1}{4} \ln(\sqrt{2} - 1) + \frac{1}{4} \ln(1 - \sqrt{\eta}) - \frac{1}{4} \ln(1 - \eta) + \frac{\ln(\eta)}{8} \right] \ln^2(2) \\
 & + \frac{\ln^3(2)}{12} - \frac{1}{4} i\pi \ln^2(\sqrt{2} - 1) + \left[ -\frac{1}{2} i\pi \ln(1 - \eta) - \frac{\ln(\eta)}{8} \right] \ln(1 - \sqrt{\eta}) \\
 & + \frac{1}{4} i\pi \ln^2(1 - \sqrt{\eta}) + \frac{1}{4} i\pi \ln^2(1 - \eta) - \frac{(1 - 3\eta)\sqrt{\eta} \ln(\eta)}{8(1 - \eta)^2} + \frac{1}{4} \text{Li}_2\left(\frac{1}{\sqrt{2}}\right) - \frac{1}{4} \text{Li}_2(\sqrt{\eta}) \\
 & + \frac{1}{2} \text{Li}_3\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{2} \text{Li}_3\left(\frac{1}{2} \left(1 + \frac{1}{\sqrt{2}}\right)\right) - \frac{1}{2} \text{Li}_3\left(1 + \frac{1}{\sqrt{2}}\right) + \frac{1}{2} \text{Li}_3\left(\frac{1}{1 + \sqrt{2}}\right) \\
 & - \frac{1}{2} \text{Li}_3\left(\frac{2}{1 + \sqrt{2}}\right) - \frac{1}{2} \text{Li}_3\left(\frac{1}{2} (1 + \sqrt{\eta})\right) + \frac{1}{2} \text{Li}_3(1 + \sqrt{\eta}) - \frac{1}{8} \text{Li}_3(1 - \eta) \\
 & \left. - \frac{1}{2} \text{Li}_3(\sqrt{\eta}) + \frac{1}{2} \text{Li}_3\left(\frac{2\sqrt{\eta}}{1 + \sqrt{\eta}}\right) \right] \tag{H.73}
 \end{aligned}$$

$$\begin{aligned}
 = & \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ \frac{1}{12} \ln^3(1 - \sqrt{\eta}) + \frac{1}{4} \ln(\eta) \text{Li}_2\left(\frac{1}{2} (1 + \sqrt{\eta})\right) + \frac{\text{Li}_2(\eta)}{16(1-\eta)^2} (1 - 2\eta + \eta^2 \right. \\
 & \left. + 4\sqrt{\eta} + 4\eta^{3/2}) - \frac{7 - 68\eta - 47\eta^2}{144(1-\eta)\sqrt{\eta}} + \left[ \frac{(1+\eta)(3 - 14\eta + 3\eta^2)}{32(1-\eta)^2\sqrt{\eta}} - \frac{1}{8\sqrt{\eta}} (3 - 2\sqrt{\eta} + 3\eta) \right. \right. \\
 & \left. \left. \times \ln(2) \right] \zeta_2 + \frac{7}{32} (1 + \sqrt{\eta})^2 \frac{\zeta_3}{\sqrt{\eta}} - \frac{1}{12} \ln^3(2) + \left[ \frac{1}{2} \zeta_2 + \frac{\ln(2)^2}{4} + \left[ -\frac{1}{8} + \frac{\ln(2)}{4} \right. \right. \right. \\
 & \left. \left. + \frac{1}{4} \ln(1 - \eta) \right] \ln(\eta) \right] \ln(1 - \sqrt{\eta}) + \left[ -\frac{\ln(2)}{4} - \frac{3\ln(\eta)}{8} \right] \ln^2(1 - \sqrt{\eta}) + \left[ \frac{(-1 + 3\eta)\sqrt{\eta}}{8(1-\eta)^2} \right. \\
 & \left. - \frac{1}{8} \zeta_2 + \frac{\ln^2(2)}{8} + \left[ \frac{1}{16(1-\eta)^2} (1 - 2\eta + \eta^2 + 4\sqrt{\eta} + 4\eta^{3/2}) - \frac{\ln(2)}{4} \right] \ln(1 - \eta) \right] \ln(\eta) \\
 & - \frac{\text{Li}_2(\sqrt{\eta})}{4} + \frac{1}{2} \text{Li}_3\left(\frac{1}{2} (1 - \sqrt{\eta})\right) - \text{Li}_3(1 - \sqrt{\eta}) + \frac{\text{Li}_3(1 - \eta)}{8} - \text{Li}_3(\sqrt{\eta}) \\
 & \left. - \frac{1}{2} \text{Li}_3\left(\frac{2\sqrt{\eta}}{-1 + \sqrt{\eta}}\right) + \frac{\text{Li}_3(\eta)}{8} \right] \tag{H.74}
 \end{aligned}$$

$$\begin{aligned}
 K_{28} & = G \left[ \left\{ -\frac{\sqrt{(1-x)x}}{\eta + x(1-\eta)}, \sqrt{(1-x)x}, \frac{1}{x} \right\}, 1 \right] \\
 & = \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ \frac{1}{4} (-1 + 2\ln(2)) \text{Li}_2\left(\frac{1}{\sqrt{2}}\right) - \frac{1}{4} \ln(2) \text{Li}_2\left(\frac{1}{2} \left(1 + \frac{1}{\sqrt{2}}\right)\right) \right. \\
 & \left. - \frac{1}{4} \ln(\eta) \text{Li}_2\left(\frac{1}{2} (1 + \sqrt{\eta})\right) + \frac{1}{4} (1 + 2\ln(\eta)) \text{Li}_2(\sqrt{\eta}) + \frac{1}{2} \text{Li}_3\left(\frac{\sqrt{\eta}}{1 + \sqrt{\eta}}\right) - \frac{c_3}{\sqrt{2}} \right]
 \end{aligned}$$

$$\begin{aligned}
 & + \frac{1}{288(1-\eta)} \left[ 317\sqrt{2}(1-\eta) - 94\frac{1}{\sqrt{\eta}} - 136\sqrt{\eta} + 14\eta^{3/2} \right] + \left( \frac{\ln(2)}{16\sqrt{\eta}} \left( 6(1+\eta) \right. \right. \\
 & \left. \left. + (3-9\sqrt{2})\sqrt{\eta} \right) + \frac{1}{64(-1+\eta)^2} \left( -6 + 22\eta + 22\eta^2 - 6\eta^3 + (2-15\sqrt{2})\sqrt{\eta} \right. \right. \\
 & \left. \left. + (-4+30\sqrt{2})\eta^{3/2} + (2-15\sqrt{2})\eta^{5/2} \right) \frac{1}{\sqrt{\eta}} + \frac{\ln(\eta)}{8} \right) \zeta_2 + \frac{7\zeta_3}{64\sqrt{\eta}} \left[ 2(1+\eta) \right. \\
 & \left. - (2+3\sqrt{2})\sqrt{\eta} \right] + \left[ \frac{1}{8}(1+2i\pi) \ln(\sqrt{2}-1) - \frac{5}{4}\frac{1}{\sqrt{2}} + \frac{1}{4} \ln^2(\sqrt{2}-1) \right. \\
 & \left. + \left( \frac{1}{2} \ln(1-\eta) - \frac{\ln(\eta)}{4} \right) \ln(1-\sqrt{\eta}) - \frac{1}{4} \ln^2(1-\sqrt{\eta}) - \frac{1}{4} \ln^2(1-\eta) \right. \\
 & \left. + \frac{1}{4} \ln(1-\eta) \ln(\eta) \right] \ln(2) + \left[ \frac{1}{32}(-1+2i\pi) + \frac{1}{8} \ln(\sqrt{2}-1) - \frac{1}{4} \ln(1-\sqrt{\eta}) \right. \\
 & \left. + \frac{1}{4} \ln(1-\eta) - \frac{\ln(\eta)}{8} \right] \ln^2(2) - \frac{1}{24} \ln^3(2) + \frac{1}{4} i\pi \ln^2(\sqrt{2}-1) + \left[ \frac{1}{2} i\pi \ln(1-\eta) \right. \\
 & \left. + \frac{\ln(\eta)}{8} + \frac{\ln^2(\eta)}{8} \right] \ln(1-\sqrt{\eta}) - \frac{1}{4} i\pi \ln^2(1-\sqrt{\eta}) + \left[ -\frac{\ln(\eta)}{16(1-\eta)^2} \left( 1-2\eta+\eta^2 \right. \right. \\
 & \left. \left. + 4\sqrt{\eta} + 4\eta^{3/2} \right) - \frac{1}{16} \ln^2(\eta) \right] \ln(1-\eta) - \frac{1}{4} i\pi \ln^2(1-\eta) - \frac{(3-\eta)\sqrt{\eta} \ln(\eta)}{8(1-\eta)^2} \\
 & + \frac{(1+\eta)\sqrt{\eta} \ln^2(\eta)}{8(1-\eta)^2} + \left[ -\frac{1}{16(1-\eta)^2} \left( 1-2\eta+\eta^2 + 4\sqrt{\eta} + 4\eta^{3/2} \right) - \frac{\ln(\eta)}{8} \right] \text{Li}_2(\eta) \\
 & + \frac{1}{2} \text{Li}_3\left(\frac{1}{\sqrt{2}}\right) - \frac{1}{2} \text{Li}_3\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) + \frac{1}{2} \text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right) - \frac{1}{2} \text{Li}_3\left(\frac{1}{1+\sqrt{2}}\right) \\
 & + \frac{1}{2} \text{Li}_3\left(\frac{2}{1+\sqrt{2}}\right) + \frac{1}{2} \text{Li}_3\left(\frac{1}{2}(1+\sqrt{\eta})\right) - \frac{1}{2} \text{Li}_3(1+\sqrt{\eta}) + \frac{1}{8} \text{Li}_3(1-\eta) \\
 & \left. - \frac{1}{2} \text{Li}_3(\sqrt{\eta}) - \frac{1}{2} \text{Li}_3\left(\frac{2\sqrt{\eta}}{1+\sqrt{\eta}}\right) + \frac{1}{8} \text{Li}_3(\eta) \right] \tag{H.75} \\
 = & \frac{\sqrt{\eta}}{(1-\eta)^2} \left[ -\frac{1}{12} \ln^3(1-\sqrt{\eta}) - \frac{1}{4} \ln(\eta) \text{Li}_2\left(\frac{1}{2}(1+\sqrt{\eta})\right) + \frac{1}{4} (1+2\ln(\eta)) \text{Li}_2(\sqrt{\eta}) \right. \\
 & \left. - \frac{47+68\eta-7\eta^2}{144(1-\eta)\sqrt{\eta}} + \left[ -\frac{(1+\eta)(3-14\eta+3\eta^2)}{32(1-\eta)^2\sqrt{\eta}} + \frac{1}{8} (3-2\sqrt{\eta}+3\eta) \ln(2) \frac{1}{\sqrt{\eta}} \right] \zeta_2 \right. \\
 & \left. + \frac{7}{32} (\sqrt{\eta}-1)^2 \frac{\zeta_3}{\sqrt{\eta}} + \frac{\ln^3(2)}{12} - \left[ \frac{1}{2} \zeta_2 + \frac{1}{4} \ln^2(2) - \left( \frac{1}{8} - \frac{\ln(2)}{4} - \frac{1}{4} \ln(1-\eta) \right) \right. \right. \\
 & \left. \left. \times \ln(\eta) - \frac{\ln^2(\eta)}{8} \right] \ln(1-\sqrt{\eta}) + \left( \frac{\ln(2)}{4} + \frac{3\ln(\eta)}{8} \right) \ln^2(1-\sqrt{\eta}) + \left[ \frac{(\eta-3)\sqrt{\eta}}{8(1-\eta)^2} \right. \right. \\
 & \left. \left. + \frac{1}{8} \zeta_2 - \frac{1}{8} \ln^2(2) - \left( \frac{1}{16(1-\eta)^2} (1-2\eta+\eta^2+4\sqrt{\eta}+4\eta^{3/2}) - \frac{\ln(2)}{4} \right) \ln(1-\eta) \right] \right. \\
 & \left. \times \ln(\eta) + \left[ \frac{(1+\eta)\sqrt{\eta}}{8(1-\eta)^2} - \frac{1}{16} \ln(1-\eta) \right] \ln^2(\eta) - \left[ \frac{1}{16(1-\eta)^2} (1-2\eta+\eta^2 \right. \right. \\
 & \left. \left. + 4\sqrt{\eta} + 4\eta^{3/2}) + \frac{\ln(\eta)}{8} \right] \text{Li}_2(\eta) - \frac{1}{2} \text{Li}_3\left(\frac{1}{2}(1-\sqrt{\eta})\right) + \text{Li}_3(1-\sqrt{\eta}) - \frac{\text{Li}_3(1-\eta)}{8} \right]
 \end{aligned}$$

$$+\frac{1}{2}\text{Li}_3\left(\frac{2\sqrt{\eta}}{-1+\sqrt{\eta}}\right)]. \quad (\text{H.76})$$

Here the constants  $c_1$  to  $c_8$  are given by

$$\begin{aligned} c_1 &= G\left[\left\{\frac{\sqrt{(1-x)x}}{1+x}, \frac{1}{x}, \sqrt{(1-x)x}\right\}, 1\right] \\ &= -\frac{17}{24} + i\frac{1}{2\sqrt{2}}\pi\ln^2(\sqrt{2}-1) + \frac{1}{2\sqrt{2}}\ln(2)\text{Li}_2\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) + \left[\frac{21}{16} - \frac{7}{8\sqrt{2}}\right]\zeta_3 \\ &\quad + \frac{5}{4}\ln(2) + \frac{1}{16\sqrt{2}}(1+2\pi i)\ln^2(2) + \frac{1}{\sqrt{2}}\ln^3(2) + \left[-\frac{15}{32} - \frac{1}{16}\frac{1}{\sqrt{2}} - \frac{1}{8}\frac{1}{\sqrt{2}}\ln(2)\right]\zeta_2 \\ &\quad - \frac{1}{\sqrt{2}}\left[\zeta_2 + \frac{1}{4}(1-2\pi i)\ln(2) + \frac{3}{8}\ln^2(2)\right]\ln(\sqrt{2}-1) - \frac{1}{6}\frac{1}{\sqrt{2}}\ln^3(\sqrt{2}-1) \\ &\quad + \frac{1}{2\sqrt{2}}\left[1-2\ln(2)\right]\text{Li}_2\left(\frac{1}{\sqrt{2}}\right) - \sqrt{2}\text{Li}_3\left(\frac{1}{\sqrt{2}}\right) - \frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{1}{2}\left(1-\frac{1}{\sqrt{2}}\right)\right) \\ &\quad + \frac{1}{\sqrt{2}}\text{Li}_3\left(1-\frac{1}{\sqrt{2}}\right) + \frac{1}{\sqrt{2}}\text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right) + \frac{1}{\sqrt{2}}\text{Li}_3\left(-\frac{2}{\sqrt{2}-1}\right) \end{aligned} \quad (\text{H.77})$$

$$\begin{aligned} c_2 &= G\left[\left\{\frac{\sqrt{(1-x)x}}{1+x}, \frac{1}{1-x}, \sqrt{(1-x)x}\right\}, 1\right] \\ &= -\frac{1}{24} - \frac{1}{2\sqrt{2}}\ln(2)\text{Li}_2\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) + \frac{1}{4\sqrt{2}}\ln(2)\text{Li}_2\left((\sqrt{2}-1)^4\right) + \left[\frac{1}{32}(3+\sqrt{2})\right. \\ &\quad \left. + \frac{7}{8\sqrt{2}}\ln(2) - \sqrt{2}\ln(\sqrt{2}-1) - \frac{3}{\sqrt{2}}\ln(1+\sqrt{2})\right]\zeta_2 + \frac{21\zeta_3}{32}(2+\sqrt{2}) + \left[-\frac{1}{4}\right. \\ &\quad \left. + \frac{1}{4\sqrt{2}}(1-2i\pi)\ln(\sqrt{2}-1)\right]\ln(2) + \left[-\frac{1}{16\sqrt{2}}(1+2i\pi) + \frac{7}{8}\frac{1}{\sqrt{2}}\ln(\sqrt{2}-1)\right]\ln(2)^2 \\ &\quad - \frac{7}{6\sqrt{2}}\ln(2)^3 - \frac{1}{2\sqrt{2}}i\pi\ln(\sqrt{2}-1)^2 + \frac{1}{6\sqrt{2}}\ln(\sqrt{2}-1)^3 - \left[\frac{1}{2\sqrt{2}} + \frac{\ln(2)}{\sqrt{2}}\right]\text{Li}_2\left(\frac{1}{\sqrt{2}}\right) \\ &\quad - \frac{1}{\sqrt{2}}\ln(2)\text{Li}_2\left((\sqrt{2}-1)^2\right) - \sqrt{2}\text{Li}_3\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{1}{2}\left(1-\frac{1}{\sqrt{2}}\right)\right) \\ &\quad - \frac{1}{\sqrt{2}}\text{Li}_3\left(1-\frac{1}{\sqrt{2}}\right) - \frac{1}{\sqrt{2}}\text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right) - \frac{1}{\sqrt{2}}\text{Li}_3\left(-\frac{2}{-1+\sqrt{2}}\right) \end{aligned} \quad (\text{H.78})$$

$$\begin{aligned} c_3 &= G\left[\left\{\frac{\sqrt{(1-x)x}}{1+x}, \sqrt{(1-x)x}, \frac{1}{x}\right\}, 1\right] \\ &= \frac{317}{144} - \frac{1}{2\sqrt{2}}\ln(2)\text{Li}_2\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) - \left[\frac{21}{32} + \frac{5}{16\sqrt{2}}\right]\zeta_3 - \frac{5}{4}\ln(2) - \frac{1}{16\sqrt{2}} \\ &\quad \times (1-2\pi i)\ln^2(2) + \frac{1}{12\sqrt{2}}\ln^3(2) + \left[-\frac{15}{32} + \frac{1}{16}\frac{1}{\sqrt{2}} - \frac{9}{8}\ln(2) - \frac{1}{8}\frac{1}{\sqrt{2}}\ln(2)\right]\zeta_2 \\ &\quad + \frac{1}{4\sqrt{2}}\left[(1+2\pi i)\ln(2) + \ln^2(2)\right]\ln(\sqrt{2}-1) + \frac{1}{2\sqrt{2}}\left[i\pi + \ln(2)\right]\ln^2(\sqrt{2}-1) \\ &\quad - \frac{1}{\sqrt{2}}\left[\frac{1}{2} - \ln(2)\right]\text{Li}_2\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{1}{\sqrt{2}}\right) - \frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) \end{aligned}$$

$$+\frac{1}{\sqrt{2}}\text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right)-\frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{1}{1+\sqrt{2}}\right)+\frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{2}{1+\sqrt{2}}\right) \quad (\text{H.79})$$

$$\begin{aligned} c_4 &= G\left[\left\{\frac{\sqrt{(1-x)x}}{1+x}, \sqrt{(1-x)x}, \frac{1}{1-x}\right\}, 1\right] \\ &= -\frac{155}{144} + \frac{1}{4}\ln(2) - \frac{3}{4}\ln^2(2) + \frac{1}{16\sqrt{2}}(1-2\pi i)\ln^2(2) + \frac{1}{2\sqrt{2}}\ln(2)\text{Li}_2\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) \\ &\quad + \left[\frac{15}{32} + \frac{9}{8}\ln(2) - \frac{1}{16}\frac{1}{\sqrt{2}} + \frac{1}{8\sqrt{2}}\ln(2)\right]\zeta_2 + \left[-\frac{21}{32} + \frac{3}{32\sqrt{2}}\right]\zeta_3 - \frac{1}{4\sqrt{2}}\left[(1+2\pi i)\ln(2)\right. \\ &\quad \left.+ 2\ln^2(2)\right]\ln(\sqrt{2}-1) - \frac{1}{2\sqrt{2}}\left[\ln(2)+i\pi\right]\ln^2(\sqrt{2}-1) + \frac{1}{2\sqrt{2}}\text{Li}_2\left(\frac{1}{\sqrt{2}}\right) \\ &\quad + \frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{1}{\sqrt{2}}\right) + \frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right) - \frac{1}{\sqrt{2}}\text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right) \\ &\quad + \frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{1}{1+\sqrt{2}}\right) - \frac{1}{\sqrt{2}}\text{Li}_3\left(\frac{2}{1+\sqrt{2}}\right), \end{aligned} \quad (\text{H.80})$$

$$\begin{aligned} c_5 &= G\left[\left\{\frac{\sqrt{(1-x)x}}{x-2}, \frac{1}{1-x}, \sqrt{(1-x)x}\right\}, 1\right] \\ &= -c_1 - \frac{3\zeta_2}{16\sqrt{2}}\left[-4+5\sqrt{2}+16\ln(2)+16\ln(\sqrt{2}-1)\right], \end{aligned} \quad (\text{H.81})$$

$$\begin{aligned} c_6 &= G\left[\left\{\frac{\sqrt{(1-x)x}}{x-2}, \frac{1}{x}, \sqrt{(1-x)x}\right\}, 1\right] \\ &= -c_2 + \frac{3\zeta_2}{16\sqrt{2}}\left[-4+\sqrt{2}+24\ln(2)+16\ln(\sqrt{2}-1)\right], \end{aligned} \quad (\text{H.82})$$

$$c_7 = G\left[\left\{\frac{\sqrt{(1-x)x}}{x-2}, \sqrt{(1-x)x}, \frac{1}{1-x}\right\}, 1\right] = -c_3 + \frac{3\zeta_2}{16}(2\sqrt{2}-3)(4\ln(2)-1), \quad (\text{H.83})$$

$$c_8 = G\left[\left\{\frac{\sqrt{(1-x)x}}{x-2}, \sqrt{(1-x)x}, \frac{1}{x}\right\}, 1\right] = -c_4 - \frac{3\zeta_2}{16}(2\sqrt{2}-3)(4\ln(2)-1). \quad (\text{H.84})$$

The following set of constants contributes in the first expressions for  $K_l$  given above.

$$\begin{aligned} &\ln(2), \pi, \ln(\sqrt{2}-1), \zeta_3, \text{Li}_2\left((\sqrt{2}-1)^2\right), \text{Li}_2\left((\sqrt{2}-1)^4\right), \text{Li}_3\left(\sqrt{2}-1\right), \\ &\text{Li}_3\left(2(\sqrt{2}-1)\right), \text{Li}_3\left(\frac{1}{2}\left(1+\frac{1}{\sqrt{2}}\right)\right), \text{Li}_3\left(1+\frac{1}{\sqrt{2}}\right), \end{aligned} \quad (\text{H.85})$$

with  $\zeta_2 = \pi^2/6$ . The new constants, most of which are not multiple zeta values [434], however, finally cancel. The first expressions were obtained by integrating using `Mathematica` and applying functional identities between (poly)logarithms [265, 266]. For the second expression, we used relations built in `HarmonicSums`. The cancellation is due to special value relations of polylogarithms. The corresponding relations may also be numerically verified, e.g. by using `PSLQ` [448].

We note the relation

$$\frac{5\zeta_2}{4} - \frac{\ln^2(2)}{4} - \ln(2)\ln\left(1+\frac{1}{\sqrt{2}}\right) + 2\text{Li}_2\left(-\frac{1}{\sqrt{2}}\right) - \text{Li}_2((\sqrt{2}-1)^2) + \text{Li}_2(-(\sqrt{2}-1)^2) = 0. \quad (\text{H.86})$$

Abel's relation for  $x = 1 - 1/\sqrt{2}$  and  $y = -1/\sqrt{2}$ , Euler's relation and the mirror relation, cf. [265,



266],

$$\operatorname{Li}_2\left(\frac{xy}{(1-x)(1-y)}\right) = \operatorname{Li}_2\left(\frac{x}{1-y}\right) + \operatorname{Li}_2\left(\frac{y}{1-x}\right) - \operatorname{Li}_2(x) - \operatorname{Li}_2(y) - \ln(1-x)\ln(1-y), \quad (\text{H.87})$$

$$\operatorname{Li}_2(1-z) = -\operatorname{Li}_2(z) - \ln(z)\ln(1-z) + \zeta_2, \quad (\text{H.88})$$

$$\operatorname{Li}_2(-z) = \frac{1}{2}\operatorname{Li}_2(z^2) - \operatorname{Li}_2(z), \quad (\text{H.89})$$

allow to rewrite

$$\operatorname{Li}_2(-(\sqrt{2}-1)^2) = -\frac{5}{4}\zeta_2 - \frac{1}{4}\ln^2(2) + \ln(2)\ln(1+\sqrt{2}) - 2\operatorname{Li}_2\left(-\frac{1}{\sqrt{2}}\right) + \operatorname{Li}_2\left((\sqrt{2}-1)^2\right), \quad (\text{H.90})$$

which proofs (H.86). The relation

$$\operatorname{H}_{0,-1,-1}(z) - \operatorname{H}_{0,-1,1}(z) - \operatorname{H}_{0,1,-1}(z) + \operatorname{H}_{0,1,1}(z) - \frac{1}{2}\operatorname{H}_{0,1,1}(z^2) = 0 \quad (\text{H.91})$$

holds. It is obtained by first considering

$$\operatorname{H}_{-1,-1}(x) - \operatorname{H}_{-1,1}(x) - \operatorname{H}_{1,-1}(x) + \operatorname{H}_{1,1}(x) = \frac{1}{2}\ln^2(1-x^2). \quad (\text{H.92})$$

The integration of the left-letter  $1/x$  then proofs (H.91). Both relations play a role in deriving the constants  $c_1$  to  $c_4$ .

Furthermore, one may use the relations

$$\begin{aligned} \operatorname{Li}_2\left(\frac{1}{2}\left(1 + \frac{1}{\sqrt{2}}\right)\right) &= -\frac{9}{8}\ln^2(2) + \frac{3}{2}\ln(2)\ln(\sqrt{2}-1) + \frac{3}{2}\ln^2(\sqrt{2}-1) \\ &\quad - \operatorname{Li}_2\left((\sqrt{2}-1)^2\right) + \frac{1}{2}\operatorname{Li}_2\left((\sqrt{2}-1)^4\right) + \zeta_2, \end{aligned} \quad (\text{H.93})$$

$$\begin{aligned} \operatorname{Li}_2\left(\frac{1}{\sqrt{2}}\right) &= \frac{7}{8}\zeta_2 - \frac{1}{8}\ln^2(2) + \frac{1}{2}\ln(2)\ln(\sqrt{2}-1) - \operatorname{Li}_2\left((\sqrt{2}-1)^2\right) \\ &\quad + \frac{1}{4}\operatorname{Li}_2\left((\sqrt{2}-1)^4\right), \end{aligned} \quad (\text{H.94})$$

$$\begin{aligned} \operatorname{Li}_2(\sqrt{2}-1) &= \operatorname{Li}_2\left(\frac{1}{\sqrt{2}}\right) - \frac{1}{4}\zeta_2 + \frac{1}{8}\ln^2(2) - \frac{1}{2}\ln(2)\ln(\sqrt{2}-1) \\ &\quad - \frac{1}{2}\ln^2(\sqrt{2}-1), \end{aligned} \quad (\text{H.95})$$

$$\operatorname{Li}_2(\sqrt{2}(\sqrt{2}-1)) = \frac{5}{4}\zeta_2 - \frac{1}{8}\ln^2(2) - \frac{1}{2}\ln^2(\sqrt{2}-1) - \operatorname{Li}_2\left(\frac{1}{\sqrt{2}}\right), \quad (\text{H.96})$$

$$\begin{aligned} \operatorname{Li}_3\left(\frac{1}{\sqrt{2}}\right) &= -\frac{5}{8}\zeta_2\ln(2) + \frac{1}{48}\ln^3(2) - \zeta_2\ln(\sqrt{2}-1) + \frac{1}{4}\ln(2)\ln^2(\sqrt{2}-1) \\ &\quad + \frac{1}{3}\ln^3(\sqrt{2}-1) + \operatorname{Li}_3(\sqrt{2}-1) + \operatorname{Li}_3(\sqrt{2}(\sqrt{2}-1)) - \frac{25}{32}\zeta_3, \end{aligned} \quad (\text{H.97})$$

$$\begin{aligned} \operatorname{Li}_3(\sqrt{2}(\sqrt{2}-1)) &= \zeta_2\ln(2) + \frac{1}{8}i\pi\ln^2(2) - \frac{1}{48}\ln^3(2) + 2\zeta_2\ln(\sqrt{2}-1) \\ &\quad + \frac{1}{2}i\pi\ln(2)\ln(\sqrt{2}-1) - \frac{1}{8}\ln^2(2)\ln(\sqrt{2}-1) + \frac{1}{2}i\pi\ln^2(\sqrt{2}-1) \end{aligned}$$

H. Identities for Encountered Iterated Integrals

$$-\frac{1}{4}\ln(2)\ln^2(\sqrt{2}-1) - \frac{1}{6}\ln^3(\sqrt{2}-1) + \text{Li}_3\left(1 + \frac{1}{\sqrt{2}}\right) \quad (\text{H.98})$$

to rewrite some of the polylogarithms above. One may finally use the relation

$$\text{Li}_3\left(\frac{1}{z}\right) = \text{Li}_3(z) + \frac{1}{6}\ln^3(z) - \frac{1}{2}i\pi\ln^2(z) - 2\zeta_2\ln(z), \quad z \in [0, 1] \quad (\text{H.99})$$

to rewrite the last two  $\text{Li}_3$ -functions in (H.86) in a more uniform way in terms of

$$\text{Li}_3(2\sqrt{2}(\sqrt{2}-1)) \quad \text{and} \quad \text{Li}_3(\sqrt{2}(\sqrt{2}-1)). \quad (\text{H.100})$$

Thus the arguments of the four trilogs contributing differ by a relative factor of  $\sqrt{2}$ . One may as well rewrite  $\text{Li}_2((\sqrt{2}-1)^2)$  and  $\text{Li}_2((\sqrt{2}-1)^4)$  into  $\text{Li}_2(2(\sqrt{2}-1))$  and  $\text{Li}_2(2\sqrt{2}(\sqrt{2}-1))$  and then obtain the set

$$\begin{aligned} &\ln(2), \pi, \ln(\sqrt{2}-1), \zeta_3, \text{Li}_2\left(2(\sqrt{2}-1)\right), \text{Li}_2\left(2\sqrt{2}(\sqrt{2}-1)\right), \\ &\text{Li}_3\left(\sqrt{2}-1\right), \text{Li}_3\left(\sqrt{2}(\sqrt{2}-1)\right), \text{Li}_3\left(2(\sqrt{2}-1)\right), \text{Li}_3\left(2\sqrt{2}(\sqrt{2}-1)\right). \end{aligned} \quad (\text{H.101})$$

# I. Fixed Moments for $A_{Qq}^{(3),\text{PS}}$

For fixed values of  $N = 2k, k \in \mathbb{N} \setminus \{0\}$  the two-mass contributions to the OME  $A_{Qq}^{(3),\text{PS}}$  can be given analytically. Using our usual conventions

$$L_1 = \ln \left( \frac{m_1^2}{\mu^2} \right), \quad L_2 = \ln \left( \frac{m_2^2}{\mu^2} \right), \quad (\text{I.1})$$

with  $\eta = m_2^2/m_1^2 < 1$ , we find the following moments:

$$\begin{aligned} \tilde{A}_{Qq}^{\text{PS},(3)}(N=2) = & -\frac{8192}{81\varepsilon^3} + \frac{1}{\varepsilon^2} \left[ -\frac{11776}{243} - \frac{2048}{27} (L_2 + L_1) \right] + \frac{1}{\varepsilon} \left[ -\frac{75136}{729} - \frac{512}{9} (L_2^2 + L_1^2) \right. \\ & - \frac{2944}{81} (L_2 + L_1) - \frac{512}{9} H_0(\eta) (L_2 - L_1) - \frac{1024}{27} H_0^2(\eta) - \frac{1024}{27} \zeta_2 \left. \right] - \frac{125600}{2187} \\ & - \frac{256}{9} (L_2^3 + L_1^3) - \frac{736}{27} (L_2^2 + L_1^2) - \frac{128}{3} H_0(\eta) (L_2^2 - L_1^2) - \left( \frac{18784}{243} + \frac{256}{9} H_0^2(\eta) \right. \\ & + \left. \frac{256}{9} \zeta_2 \right) (L_2 + L_1) - \frac{640}{27} H_0(\eta) (L_2 - L_1) + \left( -\frac{496}{81} + \frac{256}{27} H_1(\eta) \right) H_0^2(\eta) \\ & + \frac{128}{81} H_0^3(\eta) - \frac{512}{27} H_0(\eta) H_{0,1}(\eta) + \frac{512}{27} H_{0,0,1}(\eta) - \frac{1472}{81} \zeta_2 + \frac{1024}{81} \zeta_3 \\ & + \left( \frac{320}{27} + \frac{40}{27} H_0^2(\eta) \right) \left( \eta + \frac{1}{\eta} \right) + \frac{160}{27} H_0(\eta) \left( \eta - \frac{1}{\eta} \right) + \left( (32H_{0,-1}(\sqrt{\eta}) + 8H_{0,1}(\eta)) \right. \\ & \times H_0(\eta) - 4(H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) - 64H_{0,0,-1}(\sqrt{\eta}) - 8H_{0,0,1}(\eta) \left. \right) \left( \sqrt{\eta} + \frac{1}{\sqrt{\eta}} \right) \\ & + \left[ \left( \frac{160}{27} H_{0,-1}(\sqrt{\eta}) + \frac{40}{27} H_{0,1}(\eta) \right) H_0(\eta) - \frac{20}{27} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) \right. \\ & \left. - \frac{320}{27} H_{0,0,-1}(\sqrt{\eta}) - \frac{40}{27} H_{0,0,1}(\eta) \right] \left( \eta^{3/2} + \frac{1}{\eta^{3/2}} \right) \end{aligned} \quad (\text{I.2})$$

$$\begin{aligned} \tilde{A}_{Qq}^{\text{PS},(3)}(N=4) = & -\frac{30976}{2025\varepsilon^3} + \frac{1}{\varepsilon^2} \left[ -\frac{17888}{6075} - \frac{7744}{675} (L_2 + L_1) \right] + \frac{1}{\varepsilon} \left[ -\frac{6600284}{455625} - \frac{1936}{225} (L_2^2 + L_1^2) \right. \\ & - \frac{4472}{2025} (L_2 + L_1) - \frac{1936}{225} H_0(\eta) (L_2 - L_1) - \frac{3872}{675} H_0^2(\eta) - \frac{3872}{675} \zeta_2 \left. \right] - \frac{24497203}{5467500} \\ & - \frac{968}{225} (L_2^3 + L_1^3) - \frac{1118}{675} (L_2^2 + L_1^2) - \frac{484}{75} H_0(\eta) (L_2^2 - L_1^2) - \left[ \frac{1650071}{151875} + \frac{968}{225} H_0(\eta)^2 \right. \\ & + \left. \frac{968\zeta_2}{225} \right] (L_2 + L_1) - \frac{4294}{3375} H_0(\eta) (L_2 - L_1) + \left( \frac{186109}{324000} + \frac{968}{675} H_1(\eta) \right) H_0^2(\eta) \\ & + \frac{484}{2025} H_0^3(\eta) - \frac{1936}{675} H_0(\eta) H_{0,1}(\eta) + \frac{1936}{675} H_{0,0,1}(\eta) - \frac{2236}{2025} \zeta_2 + \frac{3872}{2025} \zeta_3 \end{aligned}$$

$$\begin{aligned}
& + \left( \frac{1322}{675} + \frac{1273}{5400} H_0^2(\eta) \right) \left( \eta + \frac{1}{\eta} \right) + \frac{5239}{5400} H_0(\eta) \left( \eta - \frac{1}{\eta} \right) + \left( -\frac{49}{200} - \frac{49}{1600} H_0^2(\eta) \right) \\
& \times \left( \eta^2 + \frac{1}{\eta^2} \right) - \frac{49}{400} H_0(\eta) \left( \eta^2 - \frac{1}{\eta^2} \right) + \left[ \left( \frac{39}{8} H_{0,-1}(\sqrt{\eta}) + \frac{39}{32} H_{0,1}(\eta) \right) H_0(\eta) \right. \\
& \left. - \frac{39}{64} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) - \frac{39}{4} H_{0,0,-1}(\sqrt{\eta}) - \frac{39}{32} H_{0,0,1}(\eta) \right] \left( \sqrt{\eta} + \frac{1}{\sqrt{\eta}} \right) \\
& + \left[ \left( \frac{425}{432} H_{0,-1}(\sqrt{\eta}) + \frac{425}{1728} H_{0,1}(\eta) \right) H_0(\eta) - \frac{425}{3456} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) \right. \\
& \left. - \frac{425}{216} H_{0,0,-1}(\sqrt{\eta}) - \frac{425}{1728} H_{0,0,1}(\eta) \right] \left( \eta^{3/2} + \frac{1}{\eta^{3/2}} \right) + \left( \left( -\frac{49}{400} H_{0,-1}(\sqrt{\eta}) \right. \right. \\
& \left. \left. - \frac{49}{1600} H_{0,1}(\eta) \right) H_0(\eta) + \frac{49}{3200} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) + \frac{49}{200} H_{0,0,-1}(\sqrt{\eta}) \right. \\
& \left. + \frac{49}{1600} H_{0,0,1}(\eta) \right) \left( \eta^{5/2} + \frac{1}{\eta^{5/2}} \right) \tag{I.3}
\end{aligned}$$

$$\tilde{A}_{Qq}^{PS,(3)}(N=6) =$$

$$\begin{aligned}
& - \frac{123904}{19845\epsilon^3} + \frac{1}{\epsilon^2} \left[ -\frac{121472}{297675} - \frac{30976}{6615} (L_2 + L_1) \right] + \frac{1}{\epsilon} \left[ -\frac{257649488}{43758225} - \frac{7744}{2205} (L_2^2 + L_1^2) \right. \\
& \left. - \frac{30368}{99225} (L_2 + L_1) - \frac{7744}{2205} H_0(\eta) (L_2 - L_1) - \frac{15488}{6615} H_0^2(\eta) - \frac{15488}{6615} \zeta_2 \right] - \frac{18655921961}{17503290000} \\
& - \frac{3872}{2205} (L_2^3 + L_1^3) - \frac{7592}{33075} (L_2^2 + L_1^2) - \frac{1936}{735} H_0(\eta) (L_2^2 - L_1^2) + \left( -\frac{64412372}{14586075} \right. \\
& \left. - \frac{3872}{2205} H_0^2(\eta) - \frac{3872}{2205} \zeta_2 \right) (L_2 + L_1) - \frac{2312}{9261} H_0(\eta) (L_2 - L_1) + \left( \frac{78873}{219520} + \frac{3872}{6615} H_1(\eta) \right) \\
& \times H_0^2(\eta) + \frac{1936}{19845} H_0^3(\eta) - \frac{7744}{6615} H_0(\eta) H_{0,1}(\eta) + \frac{7744}{6615} H_{0,0,1}(\eta) - \frac{15184}{99225} \zeta_2 + \frac{15488}{19845} \zeta_3 \\
& + \left( \frac{27687011}{31752000} + \frac{342121}{3386880} H_0^2(\eta) \right) \left( \eta + \frac{1}{\eta} \right) + \frac{603709}{1411200} H_0(\eta) \left( \eta - \frac{1}{\eta} \right) + \left( -\frac{5441}{23520} \right. \\
& \left. - \frac{5261}{188160} H_0^2(\eta) \right) \left( \eta^2 + \frac{1}{\eta^2} \right) - \frac{1349}{11760} H_0(\eta) \left( \eta^2 - \frac{1}{\eta^2} \right) + \left( \frac{81}{3136} + \frac{81}{25088} H_0^2(\eta) \right) \\
& \times \left( \eta^3 + \frac{1}{\eta^3} \right) + \frac{81}{6272} H_0(\eta) \left( \eta^3 - \frac{1}{\eta^3} \right) + \left[ \left( \frac{26939}{13440} H_{0,-1}(\sqrt{\eta}) + \frac{26939}{53760} H_{0,1}(\eta) \right) H_0(\eta) \right. \\
& \left. - \frac{26939}{107520} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) - \frac{26939}{6720} H_{0,0,-1}(\sqrt{\eta}) - \frac{26939}{53760} H_{0,0,1}(\eta) \right] \left( \sqrt{\eta} + \frac{1}{\sqrt{\eta}} \right) \\
& + \left[ \left( \frac{10649}{24192} H_{0,-1}(\sqrt{\eta}) + \frac{10649}{96768} H_{0,1}(\eta) \right) H_0(\eta) - \frac{10649}{193536} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) \right. \\
& \left. - \frac{10649}{12096} H_{0,0,-1}(\sqrt{\eta}) - \frac{10649}{96768} H_{0,0,1}(\eta) \right] \left( \eta^{3/2} + \frac{1}{\eta^{3/2}} \right) + \left[ \left( -\frac{223}{1920} H_{0,-1}(\sqrt{\eta}) \right. \right. \\
& \left. \left. - \frac{223}{7680} H_{0,1}(\eta) \right) H_0(\eta) + \frac{223}{15360} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) + \frac{223}{960} H_{0,0,-1}(\sqrt{\eta}) \right. \\
& \left. + \frac{223}{7680} H_{0,0,1}(\eta) \right] \left( \eta^{5/2} + \frac{1}{\eta^{5/2}} \right) + \left[ \left( \frac{81}{6272} H_{0,-1}(\sqrt{\eta}) + \frac{81}{25088} H_{0,1}(\eta) \right) H_0(\eta) \right.
\end{aligned}$$

$$\begin{aligned}
& -\frac{81}{50176} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) - \frac{81}{3136} H_{0,0,-1}(\sqrt{\eta}) - \frac{81}{25088} H_{0,0,1}(\eta) \Big] \\
& \times \left( \eta^{7/2} + \frac{1}{\eta^{7/2}} \right) \tag{I.4}
\end{aligned}$$

$$\begin{aligned}
\tilde{A}_{Qq}^{\text{PS},(3)}(N=8) = & -\frac{87616}{25515\epsilon^3} + \frac{1}{\epsilon^2} \left[ \frac{4916}{107163} - \frac{21904}{8505} (L_2 + L_1) \right] + \frac{1}{\epsilon} \left[ -\frac{33262473901}{10126903500} - \frac{5476}{2835} (L_2^2 + L_1^2) \right. \\
& + \frac{1229}{35721} (L_2 + L_1) - \frac{5476}{2835} H_0(\eta) (L_2 - L_1) - \frac{10952}{8505} H_0^2(\eta) - \frac{10952}{8505} \zeta_2 \Big] - \frac{8273033473567}{27221116608000} \\
& - \frac{2738}{2835} (L_2^3 + L_1^3) + \frac{1229}{47628} (L_2^2 + L_1^2) - \frac{1369}{945} H_0(\eta) (L_2^2 - L_1^2) + \left( -\frac{33262473901}{13502538000} \right. \\
& - \frac{2738}{2835} H_0(\eta)^2 - \frac{2738}{2835} \zeta_2 \Big) (L_2 + L_1) - \frac{40333}{510300} H_0(\eta) (L_2 - L_1) + \left( \frac{328686091}{1567641600} \right. \\
& + \frac{2738}{8505} H_1(\eta) \Big) H_0^2(\eta) + \frac{1369}{25515} H_0^3(\eta) - \frac{5476}{8505} H_0(\eta) H_{0,1}(\eta) + \frac{5476}{8505} H_{0,0,1}(\eta) + \frac{1229}{71442} \zeta_2 \\
& + \frac{10952}{25515} \zeta_3 + \left( \frac{171113081}{304819200} + \frac{4243147}{69672960} H_0^2(\eta) \right) \left( \eta + \frac{1}{\eta} \right) + \frac{4720627}{17418240} H_0(\eta) \left( \eta - \frac{1}{\eta} \right) \\
& + \left( -\frac{30598577}{108864000} - \frac{1158389}{34836480} H_0^2(\eta) \right) \left( \eta^2 + \frac{1}{\eta^2} \right) - \frac{6036587}{43545600} H_0(\eta) \left( \eta^2 - \frac{1}{\eta^2} \right) \\
& + \left( \frac{2487251}{47029248} + \frac{271091}{41803776} H_0^2(\eta) \right) \left( \eta^3 + \frac{1}{\eta^3} \right) + \frac{825131}{31352832} H_0(\eta) \left( \eta^3 - \frac{1}{\eta^3} \right) \\
& + \left( -\frac{847}{248832} - \frac{847}{1990656} H_0^2(\eta) \right) \left( \eta^4 + \frac{1}{\eta^4} \right) - \frac{847}{497664} H_0(\eta) \left( \eta^4 - \frac{1}{\eta^4} \right) \\
& + \left[ \left( \frac{48113}{43008} H_{0,-1}(\sqrt{\eta}) + \frac{48113}{172032} H_{0,1}(\eta) \right) H_0(\eta) - \frac{48113}{344064} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) \right. \\
& - \frac{48113}{21504} H_{0,0,-1}(\sqrt{\eta}) - \frac{48113}{172032} H_{0,0,1}(\eta) \Big] \left( \sqrt{\eta} + \frac{1}{\sqrt{\eta}} \right) + \left( \left( \frac{331775}{1161216} H_{0,-1}(\sqrt{\eta}) \right. \right. \\
& + \frac{331775}{4644864} H_{0,1}(\eta) \Big) H_0(\eta) - \frac{331775}{9289728} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) - \frac{331775}{580608} H_{0,0,-1}(\sqrt{\eta}) \\
& - \frac{331775}{4644864} H_{0,0,1}(\eta) \Big) \left( \eta^{3/2} + \frac{1}{\eta^{3/2}} \right) + \left[ \left( -\frac{1449}{10240} H_{0,-1}(\sqrt{\eta}) - \frac{1449}{40960} H_{0,1}(\eta) \right) H_0(\eta) \right. \\
& + \frac{1449}{81920} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) + \frac{1449}{5120} H_{0,0,-1}(\sqrt{\eta}) + \frac{1449}{40960} H_{0,0,1}(\eta) \Big] \left( \eta^{5/2} + \frac{1}{\eta^{5/2}} \right) \\
& + \left[ \left( \frac{95}{3584} H_{0,-1}(\sqrt{\eta}) + \frac{95}{14336} H_{0,1}(\eta) \right) H_0(\eta) - \frac{95}{28672} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) \right. \\
& - \frac{95}{1792} H_{0,0,-1}(\sqrt{\eta}) - \frac{95}{14336} H_{0,0,1}(\eta) \Big] \left( \eta^{7/2} + \frac{1}{\eta^{7/2}} \right) + \left( \left( -\frac{847}{497664} H_{0,-1}(\sqrt{\eta}) \right. \right. \\
& - \frac{847}{1990656} H_{0,1}(\eta) \Big) H_0(\eta) + \frac{847}{3981312} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) + \frac{847}{248832} H_{0,0,-1}(\sqrt{\eta}) \\
& + \frac{847}{1990656} H_{0,0,1}(\eta) \Big) \left( \eta^{9/2} + \frac{1}{\eta^{9/2}} \right) \tag{I.5}
\end{aligned}$$

$$\tilde{A}_{Qq}^{\text{PS},(3)}(N=10) =$$

$$\begin{aligned}
& -\frac{1605632}{735075\epsilon^3} + \frac{1}{\epsilon^2} \left[ \frac{5105152}{33078375} - \frac{401408}{245025} (L_2 + L_1) \right] + \frac{1}{\epsilon} \left[ -\frac{2689775322848}{1260782263125} - \frac{100352}{81675} (L_2^2 + L_1^2) \right. \\
& + \frac{1276288}{11026125} (L_2 + L_1) - \frac{100352}{81675} H_0(\eta) (L_2 - L_1) - \frac{200704}{245025} H_0^2(\eta) - \frac{200704}{245025} \zeta_2 \left. \right] \\
& - \frac{19054928458130951}{406677926793600000} - \frac{50176}{81675} (L_2^3 + L_1^3) + \frac{319072}{3675375} (L_2^2 + L_1^2) - \frac{25088}{27225} H_0(\eta) (L_2^2 - L_1^2) \\
& + \left( -\frac{672443830712}{420260754375} - \frac{50176}{81675} H_0^2(\eta) - \frac{50176}{81675} \zeta_2 \right) (L_2 + L_1) - \frac{436544}{13476375} H_0(\eta) (L_2 - L_1) \\
& + \left( \frac{43556878529}{331195392000} + \frac{50176}{245025} H_1(\eta) \right) H_0^2(\eta) + \frac{25088}{735075} H_0^3(\eta) - \frac{100352}{245025} H_0(\eta) H_{0,1}(\eta) \\
& + \frac{100352}{245025} H_{0,0,1}(\eta) + \frac{638144}{11026125} \zeta_2 + \frac{200704}{735075} \zeta_3 + \left( \frac{226878798767}{526901760000} + \frac{347257523}{8028979200} H_0^2(\eta) \right) \\
& \times \left( \eta + \frac{1}{\eta} \right) + \frac{2047449637}{10036224000} H_0(\eta) \left( \eta - \frac{1}{\eta} \right) + \left( -\frac{368396509553}{1075757760000} - \frac{55227289}{1405071360} H_0^2(\eta) \right) \\
& \times \left( \eta^2 + \frac{1}{\eta^2} \right) - \frac{41219216111}{245887488000} H_0(\eta) \left( \eta^2 - \frac{1}{\eta^2} \right) + \left( \frac{27528100609}{270978048000} + \frac{118201777}{9634775040} H_0^2(\eta) \right) \\
& \times \left( \eta^3 + \frac{1}{\eta^3} \right) + \frac{1819513853}{36130406400} H_0(\eta) \left( \eta^3 - \frac{1}{\eta^3} \right) + \left( -\frac{1197239}{100362240} - \frac{1182029}{802897920} H_0^2(\eta) \right) \\
& \times \left( \eta^4 + \frac{1}{\eta^4} \right) - \frac{2386873}{401448960} H_0(\eta) \left( \eta^4 - \frac{1}{\eta^4} \right) + \left( \frac{507}{991232} + \frac{507}{7929856} H_0^2(\eta) \right) \left( \eta^5 + \frac{1}{\eta^5} \right) \\
& + \frac{507}{1982464} H_0(\eta) \left( \eta^5 - \frac{1}{\eta^5} \right) + \left[ \left( \frac{980747}{1351680} H_{0,-1}(\sqrt{\eta}) + \frac{980747}{5406720} H_{0,1}(\eta) \right) H_0(\eta) \right. \\
& \left. - \frac{980747}{10813440} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) - \frac{980747}{675840} H_{0,0,-1}(\sqrt{\eta}) - \frac{980747}{5406720} H_{0,0,1}(\eta) \right] \\
& \times \left( \sqrt{\eta} + \frac{1}{\sqrt{\eta}} \right) + \left[ \left( \frac{734267}{3317760} H_{0,-1}(\sqrt{\eta}) + \frac{734267}{13271040} H_{0,1}(\eta) \right) H_0(\eta) - \frac{734267}{26542080} \right. \\
& \times (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) - \frac{734267}{1658880} H_{0,0,-1}(\sqrt{\eta}) - \frac{734267}{13271040} H_{0,0,1}(\eta) \left. \right] \\
& \times \left( \eta^{3/2} + \frac{1}{\eta^{3/2}} \right) + \left[ \left( -\frac{70889}{409600} H_{0,-1}(\sqrt{\eta}) - \frac{70889}{1638400} H_{0,1}(\eta) \right) H_0(\eta) + \frac{70889}{3276800} \right. \\
& \times (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) + \frac{70889}{204800} H_{0,0,-1}(\sqrt{\eta}) + \frac{70889}{1638400} H_{0,0,1}(\eta) \left. \right] \\
& \times \left( \eta^{5/2} + \frac{1}{\eta^{5/2}} \right) + \left[ \left( \frac{4179}{81920} H_{0,-1}(\sqrt{\eta}) + \frac{4179}{327680} H_{0,1}(\eta) \right) H_0(\eta) \right. \\
& \left. - \frac{4179}{655360} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) - \frac{4179}{40960} H_{0,0,-1}(\sqrt{\eta}) - \frac{4179}{327680} H_{0,0,1}(\eta) \right] \\
& \times \left( \eta^{7/2} + \frac{1}{\eta^{7/2}} \right) + \left[ \left( -\frac{39641}{6635520} H_{0,-1}(\sqrt{\eta}) - \frac{39641}{26542080} H_{0,1}(\eta) \right) H_0(\eta) \right. \\
& \left. + \frac{39641}{53084160} (H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta})) H_0^2(\eta) + \frac{39641}{3317760} H_{0,0,-1}(\sqrt{\eta}) + \frac{39641}{26542080} H_{0,0,1}(\eta) \right] \\
& \times \left( \eta^{9/2} + \frac{1}{\eta^{9/2}} \right) + \left[ \left( \frac{507}{1982464} H_{0,-1}(\sqrt{\eta}) + \frac{507}{7929856} H_{0,1}(\eta) \right) H_0(\eta) - \frac{507}{15859712} \right.
\end{aligned}$$

$$\begin{aligned} & \times \left( H_{-1}(\sqrt{\eta}) + H_1(\sqrt{\eta}) \right) H_0^2(\eta) - \frac{507}{991232} H_{0,0,-1}(\sqrt{\eta}) - \frac{507}{7929856} H_{0,0,1}(\eta) \Big] \\ & \times \left( \eta^{11/2} + \frac{1}{\eta^{11/2}} \right). \end{aligned} \tag{I.6}$$

This fixed moments can be used to check the momentum space result given in Chapter 7.1 without any approximation in  $\eta$ .





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