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Mellin moments of the $O(\alpha_s^3)$ heavy flavor contributions to unpolarized deep-inelastic scattering at $Q^2 \gg m^2$ and anomalous dimensions

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Abstract

We calculate the $O(\alpha_s^3)$ heavy flavor contributions to the Wilson coefficients of the structure function $F_2(x, Q^2)$ and the massive operator matrix elements (OMEs) for the twist-2 operators of unpolarized deeply inelastic scattering in the region $Q^2 \gg m^2$. The massive Wilson coefficients are obtained as convolutions of massive OMEs and the known light flavor Wilson coefficients. We also compute the massive OMEs which are needed to evaluate heavy flavor parton distributions in the variable flavor number scheme (VFNS) to 3-loop order. All contributions to the Wilson coefficients and operator matrix elements but the genuine constant terms at $O(\alpha_s^3)$ of the OMEs are derived in terms of quantities, which are known for general values in the Mellin variable N. For the operator matrix elements $A_{Qg}^{(3)}$, $A_{qg,Q}^{(3)}$ and $A_{gg,Q}^{(3)}$ the moments $N = 2$–10, for $A_{Qq}^{(3),\mathrm{PS}}$ to $N = 12$, and for $A_{qq,Q}^{(3),\mathrm{NS}}$, $A_{qq,Q}^{(3),\mathrm{PS}}$, $A_{gq,Q}^{(3)}$ to $N = 14$ are computed. These terms contribute to the light flavor $+$-combinations. For the flavor non-singlet terms, we calculate as well the odd moments $N = 1$–13, corresponding to the light flavor $-$-combinations. We also obtain the moments of the 3-loop anomalous dimensions, their color projections for the present processes respectively, in an independent calculation, which agree with the results given in the literature.

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1. Introduction

Deep-inelastic scattering processes of charged or neutral leptons off proton and deuteron targets, in the region of large enough values of the gauge boson virtuality $Q^2 = -q^2$ and hadronic mass $W^2 = (q + p)^2$, allow to measure the leading twist parton densities of the nucleon, the QCD-scale Λ_{QCD} and the strong coupling constant $a_s(Q^2) = \alpha_s(Q^2)/(4\pi)$, to high precision. The precise value of Λ_{QCD}, a fundamental parameter of the Standard Model, is of central importance for the quantitative understanding of all strongly interacting processes. Moreover, the possible unification of the gauge forces [1] depends crucially on its value. Of similar importance is the detailed knowledge of the parton densities for all hadron-induced processes [2], notably for the interpretation of all scattering cross sections measured at the Tevatron and the LHC. For example, the process of Higgs-boson production at the LHC [3] depends on the gluon density and its accuracy is widely determined by this distribution.

Let us consider the kinematic region in deeply inelastic scattering, where processes of higher twist can be safely disregarded and the hard scales Q^2 and W^2 are large enough to allow the application of the light-cone expansion, saturated by the twist-2 contributions. The scattering processes are then described by structure functions $F_i(x, Q^2)$, which decompose into *non-perturbative massless* parton densities $f_j(x, \mu^2)$ and *perturbative* coefficient functions $C_i^j(x, Q^2/\mu^2)$ by

$$F_i\left(x, Q^2\right) = \sum_{j=q,\bar{q},g} C_i^j\left(x, \frac{Q^2}{\mu^2}\right) \otimes f_j\left(x, \mu^2\right). \tag{1.1}$$

The scale μ denotes the factorization scale, which is arbitrary and cancels between the coefficient functions and parton distribution functions in the respective orders in perturbation theory. The symbol $\otimes$ denotes the Mellin convolution

$$[A \otimes B](x) = \int_0^1 dx_1 \int_0^1 dx_2\, \delta(x - x_1 x_2) A(x_1) B(x_2). \tag{1.2}$$

The Mellin transformation

$$\boldsymbol{M}\left[f(x)\right](N) = \int_0^1 dx\, x^{N-1} f(x), \tag{1.3}$$

if applied to (1.2), resolves the convolution into a product.

Since we strictly consider twist-2 collinear parton densities in the Bjorken limit, no transverse momentum effects in the initial distributions will be allowed, which otherwise is related in the kinematic sense to higher twist operators. As is well known, the leading-twist approximation and the QCD improved parton model are equivalent descriptions for the dominant contributions to the deep-inelastic structure functions at sufficiently large scales Q^2. The condition for the validity of the parton model [4] demands that

$$\frac{\tau_{\mathrm{int}}}{\tau_{\mathrm{life}}} \ll 1, \tag{1.4}$$

with τ_{int} being the interaction time of the virtual gauge boson with a hadronic quantum-fluctuation, the life-time of which is given by τ_{life}. The latter can be interpreted as a partonic state, provided (1.4) holds. Both times are measured in an infinite momentum frame and they are given by

$$\tau_{\rm int} \sim \frac{1}{q_0} = \frac{4Px}{Q^2(1-x)}, \tag{1.5}$$

$$\tau_{\rm life} \sim \frac{1}{\sum_i E_i - E} = \frac{2P}{\sum_i (k_{\perp,i}^2 + m_i^2)/x_i - M_N^2}, \qquad \sum_i x_i = 1, \tag{1.6}$$

with P the large momentum of the hadron, q_0 the energy component of the virtual gauge boson in the infinite momentum frame, E_i the energy of the ith fluctuating parton, $k_{\perp,i}$, m_i, x_i its transverse momentum, mass, and momentum fraction, E the total energy, and M_N the nucleon mass. In the region of not too small values, nor values near the elastic region $x \simeq 1$, of the Bjorken variable x, the partonic description holds for massless partons. Evidently, for the production of a heavy quark pair near threshold their kinematics *is not collinear* to the 'mother'-parton and the nucleon, due to the missing boost. We will discuss later (Section 6) under which conditions one may define heavy quark parton densities within the variable flavor scheme.

To perform the perturbative calculation we will first refer to the fixed-flavor number scheme and start with strictly massless (longlived) partonic states to obey a LSZ-requirement.[1] Within this framework one separates the light, $C_i^{j,\rm light}$, and the heavy flavor contributions, H_i^j, to the Wilson coefficients,

$$C_i^j\left(x, \frac{Q^2}{\mu^2}, \frac{m_k^2}{\mu^2}\right) = C_i^{j,\rm light}\left(x, \frac{Q^2}{\mu^2}\right) + \mathsf{H}_i^j\left(x, \frac{Q^2}{\mu^2}, \frac{m_k^2}{\mu^2}\right), \quad k = c, b, \tag{1.7}$$

with

$$\mathsf{H}_i^j\left(x, \frac{Q^2}{\mu^2}, \frac{m_k^2}{\mu^2}\right) = \mathsf{H}_i^{j,\mathsf{asymp}}\left(x, \frac{Q^2}{\mu^2}, \frac{m_k^2}{\mu^2}\right) + \mathsf{H}_i^{j,\mathsf{power}}\left(x, \frac{Q^2}{\mu^2}, \frac{m_k^2}{\mu^2}\right), \tag{1.8}$$

where the first term describes all logarithmic and the constant contribution in m_k^2/μ^2, cf. (2.11)–(2.15), and the second term the power corrections $(m_k^2/\mu^2)^l$, $l \geqslant 1$. Both, the measurements of the heavy flavor part of the deep-inelastic structure functions, cf. [5], and numerical studies [6] based on the leading [7] and next-to-leading order (NLO) heavy flavor Wilson coefficients [8], show that the scaling violations of the light and the heavy contributions to (1.7) exhibit a different behaviour over a wide range of Q^2. This is both due to the logarithmic contributions $\ln^k(Q^2/m^2)$ and power corrections $\propto (m^2/Q^2)^k$, $k \geqslant 1$. Moreover, in the region of smaller values of x the heavy flavor contributions amount to 20–40%. Therefore, the precision measurement of the QCD parameter $\Lambda_{\rm QCD}$ [9] and the parton distribution functions in deeply inelastic scattering require the description of the light and heavy flavor contributions at the same accuracy. The separation (1.7) allows the definition of the light flavor contributions and the related heavy flavor contributions to $F_i(x, Q^2)$ applying the factorization Eq. (1.1).

The perturbative accuracy reached for $F_i^{\rm light}(x, Q^2)$ is of 3-loop order [10–26], which requires to calculate the 3-loop heavy flavor Wilson coefficients as well. The NLO heavy flavor corrections in the complete kinematic range are available only in semi-analytic form [8] due

[1] We are aware that due to color confinement, this is an idealized picture. On the other hand, after having performed factorization, this is the only way in which a consistent calculation can be carried out.

to the complexity of the contributing phase space integrals.[2] Heavy flavor corrections to different sum rules for deep-inelastic structure functions were calculated in [28]. An important part of the kinematic region is that of larger values of Q^2. As has been shown in Ref. [29], the heavy flavor Wilson coefficients $\mathsf{H}_2^j(x, Q^2/\mu^2, m_i^2/\mu^2)$ can be calculated analytically at NLO for $Q^2/m^2 \gtrsim 10$.[3] This is due to a factorization of the heavy quark Wilson coefficients into massive OMEs, A_{jk}, and massless Wilson coefficients, $C_i^{j,\text{light}}$ in case one heavy quark flavor of mass m and n_f light flavors are considered. This restriction to only one heavy quark flavor is required beginning with the 3-loop corrections and will be adopted in the following. In the present paper, we calculate the massive operator matrix elements A_{jk} contributing to the heavy flavor Wilson coefficients for the structure function $F_2(x, Q^2)$ in the region $Q^2/m^2 \gtrsim 10$ to 3-loop order for fixed moments of the Mellin variable N. In case of the flavor non-singlet (NS) contributions, we also present the odd moments of the $-$-projection. We further calculate the operator matrix elements, which are required to define heavy quark densities in the VFNS [31]. Due to renormalization, higher order contributions in ε to corrections of lower order in a_s, cf. [29,31–35], and other renormalization terms, such as the anomalous dimensions and the expansion coefficients of the QCD β-function and mass anomalous dimensions, contribute. For these reasons, the present calculation yields also the moments of the complete 2-loop anomalous dimensions and the terms $\propto T_F$ of the 3-loop anomalous dimensions $\gamma_{ij}(N)$. In the pure singlet (PS) case, $\gamma_{qq}^{+,\mathsf{PS}}(N)$, and for $\gamma_{qg}(N)$, these are the complete anomalous dimensions given in [18,19], to which we agree. Since the present calculation is completely independent by method, formalism, and codes, it provides a check on the previous results. Except for the constant part of the unrenormalized heavy flavor operator matrix elements, we obtain the heavy quark Wilson coefficients in the asymptotic region for all values of the Mellin variable N. The analytic continuation of these expressions to complex values of N can be performed with the help of the representations in [36] and those given for the anomalous dimensions and massless Wilson coefficients in [18,19,26].

The paper is organized as follows. In Section 2, a brief outline of the basic formalism is given. The renormalization of the different massive operator matrix elements is described in Section 3. In Section 4, we present details on the unrenormalized and renormalized operator matrix elements. Technical details of the calculation and the main results are discussed in Section 5. Depending on the CPU time and storage size required, the moments up to $N = 10$, 12, and 14 of the different operator matrix elements could be calculated. In Section 6, representations for heavy quark parton densities in the region $\mu^2 \gg m^2$ are given and Section 7 contains the conclusions. In Appendix A, we give a consistent set of Feynman rules for the composite operators up to 3-loop order, present the moments of the 3-loop anomalous dimensions, and of the constants part of the different 3-loop massive operator matrix elements.

2. The formalism

The heavy quark contribution to the structure function $F_2(x, Q^2)$ for one heavy flavor of mass m and n_f light flavors is given by [31],

[2] A precise numerical implementation in Mellin space was given in [27].

[3] In case of $\mathsf{H}_L^j(x, Q^2/\mu^2, m_i^2/\mu^2)$ this approximation is only valid for $Q^2/m^2 \gtrsim 800$ [29]. The 3-loop corrections were calculated in Ref. [30].

$$
\begin{aligned}
&F_{2,Q}\big(x,Q^2,n_f,m\big)\\
&\quad=\sum_{k=1}^{n_f} e_k^2\Biggl\{L_{2,q}^{\mathsf{NS}}\left(n_f,\frac{Q^2}{m^2},\frac{m^2}{\mu^2}\right)\otimes\left[f_k\big(x,\mu^2,n_f\big)+f_{\bar k}\big(x,\mu^2,n_f\big)\right]\\
&\qquad+\tilde L_{2,q}^{\mathsf{PS}}\left(n_f,\frac{Q^2}{m^2},\frac{m^2}{\mu^2}\right)\otimes\Sigma\big(x,\mu^2,n_f\big)+\tilde L_{2,g}^{\mathsf{S}}\left(n_f,\frac{Q^2}{m^2},\frac{m^2}{\mu^2}\right)\otimes G\big(x,\mu^2,n_f\big)\Biggr\}\\
&\qquad+e_Q^2\Biggl[H_{2,q}^{\mathsf{PS}}\left(n_f,\frac{Q^2}{m^2},\frac{m^2}{\mu^2}\right)\otimes\Sigma\big(x,\mu^2,n_f\big)\\
&\qquad+H_{2,g}^{\mathsf{S}}\left(n_f,\frac{Q^2}{m^2},\frac{m^2}{\mu^2}\right)\otimes G\big(x,\mu^2,n_f\big)\Biggr],
\end{aligned}
\tag{2.1}
$$

with (S) the singlet contributions. Here, we denote the heavy flavor Wilson coefficients H_i^j by L_i^j, H_i^j respectively, depending on whether the photon couples to a light (L) or the heavy (H) quark line. $f_k(x,\mu^2)$ and $f_{\bar k}(x,\mu^2)$ denote the quark- and antiquark-distribution functions, $G(x,\mu^2)$ is the gluon distribution and

$$
\Sigma\big(x,\mu^2\big)=\sum_{k=1}^{n_f}\left[f_k\big(x,\mu^2\big)+f_{\bar k}\big(x,\mu^2\big)\right]
\tag{2.2}
$$

denotes the flavor singlet distribution. e_Q is the electric charge of the heavy quark. Due to the difference of quantities taken at n_f+1 and n_f flavors, it is useful to adopt the following notation for a function $f(n_f)$,

$$
\hat f(n_f)\equiv f(n_f+1)-f(n_f),
\tag{2.3}
$$

$$
\tilde f(n_f)\equiv\frac{f(n_f)}{n_f},
\tag{2.4}
$$

and $\hat{\tilde f}(n_f)\equiv[\widehat{\tilde f(n_f)}]$.[4] As has been shown in Ref. [29], the heavy quark Wilson coefficients in deeply-inelastic scattering, H_i^j, factorize in the region $Q^2\gg m^2$, in which power corrections can be disregarded, into massive operator matrix elements $A_{kl}^{\mathsf{NS,S}}$ and the light flavor Wilson coefficients $C_{i,k}^{\mathsf{NS,S}}$,

$$
\mathsf{H}_{i,l}^{\mathsf{NS,S}}=A_{kl}^{\mathsf{NS,S}}\otimes C_{i,k}^{\mathsf{NS,S}},
\tag{2.5}
$$

where $i=2,L$ specifies the structure function considered.

The operator matrix elements $A_{k,l}^{\mathsf{NS,S}}$ are the partonic expectation values

$$
A_{kl}^{\mathsf{NS,S}}\left(N,\frac{m^2}{\mu^2}\right)=\langle l|O_k^{\mathsf{NS,S}}|l\rangle,\quad l=q,g,
\tag{2.6}
$$

with the local twist-2 operators given by

$$
O_{F,a;\mu_1,\ldots,\mu_n}^{\mathsf{NS}}=i^{n-1}\mathbf{S}\left[\bar\psi\gamma_{\mu_1}D_{\mu_2}\cdots D_{\mu_n}\frac{\lambda_a}{2}\psi\right]-\text{trace terms},
\tag{2.7}
$$

[4] Later on, the symbol ˆ will also be used for the bare coupling $\hat a_s$, the mass $\hat m$, and the bare OMEs, where (2.3) is not applied.

$$O^{\mathsf{S}}_{F;\mu_1,\ldots,\mu_n} = i^{n-1}\mathbf{S}[\bar{\psi}\gamma_{\mu_1}D_{\mu_2}\cdots D_{\mu_n}\psi] - \text{trace terms}, \tag{2.8}$$

$$O^{\mathsf{S}}_{V;\mu_1,\ldots,\mu_n} = 2i^{n-2}\mathbf{SSp}\big[F^a_{\mu_1\alpha}D_{\mu_2}\cdots D_{\mu_{n-1}}F^{\alpha,a}_{\mu_n}\big] - \text{trace terms}, \tag{2.9}$$

for the fermionic non-singlet, singlet, and gluonic case [37]. Here, **S** denotes the symmetrization operator of the Lorentz indices $\mu_1,\ldots,\mu_n$; λ_a is the flavor matrix of $SU(n_f)$ with n_f light flavors, ψ denotes the quark field, $F^a_{\mu\nu}$ the gluon field-strength tensor, and D_μ the covariant derivative. **Sp** in (2.9) is the color-trace. The quarkonic operator matrix element can be represented by

$$A^{\mathsf{S}}_{qq} = A^{\mathsf{NS}}_{qq} + A^{\mathsf{PS}}_{qq}. \tag{2.10}$$

The different contributions to (2.5) were given in [31, Eqs. (2.31)–(2.35)]. To $O(a_s^3)$, the Wilson coefficients H_i^j in Mellin space are:

$$\begin{aligned} L^{\mathsf{NS}}_{2,q}(n_f) &= a_s^2\big[A^{\mathsf{NS},(2)}_{qq,Q}(n_f) + \hat{C}^{\mathsf{NS},(2)}_{2,q}(n_f)\big] \\ &\quad + a_s^3\big[A^{\mathsf{NS},(3)}_{qq,Q}(n_f) + A^{\mathsf{NS},(2)}_{qq,Q}(n_f)C^{\mathsf{NS},(1)}_{2,q}(n_f) + \hat{C}^{\mathsf{NS},(3)}_{2,q}(n_f)\big], \end{aligned} \tag{2.11}$$

$$\tilde{L}^{\mathsf{PS}}_{2,q}(n_f) = a_s^3\big[\tilde{A}^{\mathsf{PS},(3)}_{qq,Q}(n_f) + A^{(2)}_{gq,Q}(n_f)\tilde{C}^{(1)}_{2,g}(n_f+1) + \hat{\tilde{C}}^{\mathsf{PS},(3)}_{2,q}(n_f)\big], \tag{2.12}$$

$$\begin{aligned} \tilde{L}^{\mathsf{S}}_{2,g}(n_f) &= a_s^2 A^{(1)}_{gg,Q}(n_f)\tilde{C}^{(1)}_{2,g}(n_f+1) \\ &\quad + a_s^3\big[\tilde{A}^{(3)}_{qg,Q}(n_f) + A^{(1)}_{gg,Q}(n_f)\tilde{C}^{(2)}_{2,g}(n_f+1) + A^{(2)}_{gg,Q}(n_f)\tilde{C}^{(1)}_{2,g}(n_f+1) \\ &\quad + A^{(1)}_{Qg}(n_f)\tilde{C}^{\mathsf{PS},(2)}_{2,q}(n_f+1) + \hat{\tilde{C}}^{(3)}_{2,g}(n_f)\big], \end{aligned} \tag{2.13}$$

$$\begin{aligned} H^{\mathsf{PS}}_{2,q}(n_f) &= a_s^2\big[A^{\mathsf{PS},(2)}_{Qq}(n_f) + \tilde{C}^{\mathsf{PS},(2)}_{2,q}(n_f+1)\big] \\ &\quad + a_s^3\big[A^{\mathsf{PS},(3)}_{Qq}(n_f) + \tilde{C}^{\mathsf{PS},(3)}_{2,q}(n_f+1) + A^{(2)}_{gq,Q}(n_f)\tilde{C}^{(1)}_{2,g}(n_f+1) \\ &\quad + A^{\mathsf{PS},(2)}_{Qq}(n_f)C^{\mathsf{NS},(1)}_{2,q}(n_f+1)\big], \end{aligned} \tag{2.14}$$

$$\begin{aligned} H^{\mathsf{S}}_{2,g}(n_f) &= a_s\big[A^{(1)}_{Qg}(n_f) + \tilde{C}^{(1)}_{2,g}(n_f+1)\big] \\ &\quad + a_s^2\big[A^{(2)}_{Qg}(n_f) + A^{(1)}_{Qg}(n_f)C^{\mathsf{NS},(1)}_{2,q}(n_f+1) + A^{(1)}_{gg,Q}(n_f)\tilde{C}^{(1)}_{2,g}(n_f+1) \\ &\quad + \tilde{C}^{(2)}_{2,g}(n_f+1)\big] \\ &\quad + a_s^3\big[A^{(3)}_{Qg}(n_f) + A^{(2)}_{Qg}(n_f)C^{\mathsf{NS},(1)}_{2,q}(n_f+1) + A^{(2)}_{gg,Q}(n_f)\tilde{C}^{(1)}_{2,g}(n_f+1) \\ &\quad + A^{(1)}_{Qg}(n_f)\big[C^{\mathsf{NS},(2)}_{2,q}(n_f+1) + \tilde{C}^{\mathsf{PS},(2)}_{2,q}(n_f+1)\big] + A^{(1)}_{gg,Q}(n_f)\tilde{C}^{(2)}_{2,g}(n_f+1) \\ &\quad + \tilde{C}^{(3)}_{2,g}(n_f+1)\big]. \end{aligned} \tag{2.15}$$

For brevity, we have dropped here part of the arguments of the Wilson coefficients and operator matrix elements by identifying $\mathsf{H}_i^j = \mathsf{H}_i^j(N, Q^2/\mu^2, \mu^2/m^2, n_f)$, $C_i^j = C_i^j(N, Q^2/\mu^2, n_f)$ and $A_{ij} = A_{ij}(N, m^2/\mu^2, n_f)$. These representations were verified in the LO and NLO case comparing with the results in [7,8] for $Q^2 \gg m^2$.

The massive operator matrix elements are calculated keeping the external massless parton lines on-shell, while the heavy quark mass m sets the scale. The massless Wilson coefficients C_i^j in (2.11)–(2.15) were calculated in Refs. [20,21,23–26].

3. Renormalization of the massive operator matrix elements

We perform the calculation of the massive operator matrix elements in $D = 4 + \varepsilon$ dimensions and apply dimensional regularization. For each loop integral a factor S_ε

$$S_\varepsilon = \exp\left[\frac{\varepsilon}{2}\big(\gamma_E - \ln(4\pi)\big)\right], \tag{3.1}$$

with γ_E the Euler–Mascheroni constant, is obtained which collects universal terms, and $S_\varepsilon := 1$ in the $\overline{\mathsf{MS}}$-scheme. The following equation shows the perturbative expansion of the unrenormalized OMEs, denoted by a double-hat, in the bare coupling constant $\hat{a}_s$ in Mellin space

$$\begin{aligned}\hat{\hat{A}}_{ij}\left(\frac{\hat{m}^2}{\mu^2}, \varepsilon, N\right) &= \delta_{ij} + \sum_{l=1}^{\infty} \hat{a}_s^l \hat{\hat{A}}_{ij}^{(l)}\left(\frac{\hat{m}^2}{\mu^2}, \varepsilon, N\right) \\ &= \delta_{ij} + \sum_{l=1}^{\infty} \hat{a}_s^l \left(\frac{\hat{m}^2}{\mu^2}\right)^{l\varepsilon/2} \hat{\hat{A}}_{ij}^{(l)}\big(\hat{m}^2 = \mu^2, \varepsilon, N\big),\end{aligned} \tag{3.2}$$

with

$$\hat{\hat{A}}_{ij}^{(l)}\big(\hat{m}^2 = \mu^2, \varepsilon, N\big) = \sum_{k=0}^{\infty} \frac{1}{\varepsilon^{l-k}} a_{ij}^{(l,k)}(N). \tag{3.3}$$

Here, N is the Mellin-parameter, (1.3), $\hat{m}$ the bare mass, and $\mu = \mu_R$ is the renormalization scale. Also the factorization scale μ_F will be identified with μ in the following.

The factorization between the massive OMEs and the massless Wilson coefficients (2.5) requires the external legs of the operator matrix elements to be on-shell,

$$p^2 = 0, \tag{3.4}$$

where p denotes the external momentum. Unlike in the massless case, where the scale of the OMEs is set by an off-shell momentum $-p^2 < 0$, in our framework the internal heavy quark mass sets the scale. In the former case, one observes a mixing of the physical OMEs with non-gauge invariant (NGI) operators, cf. [16,38,39], and contributions originating in the violation of the equations of motion (EOM). Terms of this kind do not contribute in the present case.

The renormalization of the massive OMEs is performed in four steps. First mass renormalization is carried out, for which we use the on-mass-shell scheme and later also compare to the results in the $\overline{\mathsf{MS}}$-scheme. Afterwards, charge renormalization is performed in the $\overline{\mathsf{MS}}$-scheme. To maintain condition (3.4), which is of physical importance, we will, however, first introduce a MOM-scheme for the strong coupling constant and then perform a finite renormalization changing to the $\overline{\mathsf{MS}}$-scheme. The former scheme is implied by keeping the external massless parton lines on shell. Note, that there are other, differing MOM-schemes in the literature, cf. e.g. [40]. After mass and coupling constant renormalization, the OMEs are denoted by a single hat, $\hat{A}_{ij}$. The ultraviolet singularities of the composite operators are canceled via the corresponding Z_{ij}-factors and the UV-finite OMEs are denoted by a double tilde, $\tilde{\tilde{A}}_{ij}$. Finally, the collinear divergences are removed via mass factorization.

3.1. Mass renormalization

There are two main schemes to perform mass renormalization: (i) the on-shell scheme and (ii) the $\overline{\mathsf{MS}}$-scheme. We will apply the on-shell scheme in the following, defining the heavy quark mass as the pole mass, and compare to the $\overline{\mathsf{MS}}$-scheme later. The bare mass in (3.2) is replaced by the on-shell mass m through

$$\hat{m} = Z_m m = m\left[1 + \hat{a}_s\left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2}\delta m_1 + \hat{a}_s^2\left(\frac{m^2}{\mu^2}\right)^{\varepsilon}\delta m_2\right] + O\left(\hat{a}_s^3\right). \tag{3.5}$$

The constants in the above equation are [5]

$$\delta m_1 = C_F\left[\frac{6}{\varepsilon} - 4 + \left(4 + \frac{3}{4}\zeta_2\right)\varepsilon\right] \tag{3.6}$$

$$\equiv \frac{\delta m_1^{(-1)}}{\varepsilon} + \delta m_1^{(0)} + \delta m_1^{(1)}\varepsilon, \tag{3.7}$$

$$\begin{aligned}\delta m_2 = C_F\Bigg[&\frac{1}{\varepsilon^2}\left(18C_F - 22C_A + 8T_F(n_f + N_h)\right)\\ &+ \frac{1}{\varepsilon}\left(-\frac{45}{2}C_F + \frac{91}{2}C_A - 14T_F(n_f + N_h)\right)\\ &+ C_F\left(\frac{199}{8} - \frac{51}{2}\zeta_2 + 48\ln(2)\zeta_2 - 12\zeta_3\right)\\ &+ C_A\left(-\frac{605}{8} + \frac{5}{2}\zeta_2 - 24\ln(2)\zeta_2 + 6\zeta_3\right)\\ &+ T_F\left[n_f\left(\frac{45}{2} + 10\zeta_2\right) + N_h\left(\frac{69}{2} - 14\zeta_2\right)\right]\Bigg]\end{aligned} \tag{3.8}$$

$$\equiv \frac{\delta m_2^{(-2)}}{\varepsilon^2} + \frac{\delta m_2^{(-1)}}{\varepsilon} + \delta m_2^{(0)}, \tag{3.9}$$

with $C_F = (N_c^2 - 1)/(2N_c)$, $C_A = N_c$, $T_F = 1/2$ for $SU(N_c)$ and $N_c = 3$ in case of QCD. ζ_k denotes the Riemann ζ-function. In (3.8), n_f denotes the number of light flavors and N_h the number of heavy flavors, which we will set equal to one from now on. The pole terms were given in [41,42], and the constant term in [43,44], see also [45]. In Eqs. (3.7), (3.9), we have defined the expansion coefficients in ε of the corresponding quantities. The following equation shows the general structure of the OMEs up to $O(\hat{a}_s^3)$ after mass renormalization

$$\begin{aligned}\hat{A}_{ij}\left(\frac{m^2}{\mu^2}, \varepsilon, N\right) = \delta_{ij} &+ \hat{a}_s \hat{\hat{A}}_{ij}^{(1)}\left(\frac{m^2}{\mu^2}, \varepsilon, N\right)\\ &+ \hat{a}_s^2\left[\hat{\hat{A}}_{ij}^{(2)}\left(\frac{m^2}{\mu^2}, \varepsilon, N\right) + \delta m_1\left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} m\frac{d}{dm}\hat{\hat{A}}_{ij}^{(1)}\left(\frac{m^2}{\mu^2}, \varepsilon, N\right)\right]\\ &+ \hat{a}_s^3\left[\hat{\hat{A}}_{ij}^{(3)}\left(\frac{m^2}{\mu^2}, \varepsilon, N\right) + \delta m_1\left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} m\frac{d}{dm}\hat{\hat{A}}_{ij}^{(2)}\left(\frac{m^2}{\mu^2}, \varepsilon, N\right)\right.\\ &+ \delta m_2\left(\frac{m^2}{\mu^2}\right)^{\varepsilon} m\frac{d}{dm}\hat{\hat{A}}_{ij}^{(1)}\left(\frac{m^2}{\mu^2}, \varepsilon, N\right)\\ &\left.+ \frac{\delta m_1^2}{2}\left(\frac{m^2}{\mu^2}\right)^{\varepsilon} m^2\frac{d^2}{dm^2}\hat{\hat{A}}_{ij}^{(1)}\left(\frac{m^2}{\mu^2}, \varepsilon, N\right)\right].\end{aligned} \tag{3.10}$$

[5] Note that there is a misprint in the double-pole term of Eq. (28) in Ref. [34].

3.2. Renormalization of the coupling

As the next step, we consider charge renormalization. We briefly summarize first the main steps in the massless case in the $\overline{\mathsf{MS}}$-scheme. Afterwards, we extend the description to the massive case in the MOM-scheme which we use, before we transform back to the $\overline{\mathsf{MS}}$-scheme.

The bare coupling constant $\hat{a}_s$ is expressed by the renormalized coupling $a_s^{\overline{\mathsf{MS}}}$ via

$$\begin{aligned}\hat{a}_s &= Z_g^{\overline{\mathsf{MS}}^2}(\varepsilon, n_f) a_s^{\overline{\mathsf{MS}}}(\mu^2) \\ &= a_s^{\overline{\mathsf{MS}}}(\mu^2)\left[1 + \delta a_{s,1}^{\overline{\mathsf{MS}}}(n_f) a_s^{\overline{\mathsf{MS}}}(\mu^2) + \delta a_{s,2}^{\overline{\mathsf{MS}}}(n_f) a_s^{\overline{\mathsf{MS}}^2}(\mu)\right] + O\left(a_s^{\overline{\mathsf{MS}}^3}\right).\end{aligned} \tag{3.11}$$

The coefficients in Eq. (3.11) are [46–49] and [50,51],

$$\delta a_{s,1}^{\overline{\mathsf{MS}}}(n_f) = \frac{2}{\varepsilon}\beta_0(n_f), \tag{3.12}$$

$$\delta a_{s,2}^{\overline{\mathsf{MS}}}(n_f) = \frac{4}{\varepsilon^2}\beta_0^2(n_f) + \frac{1}{\varepsilon}\beta_1(n_f), \tag{3.13}$$

with

$$\beta_0(n_f) = \frac{11}{3}C_A - \frac{4}{3}T_F n_f, \tag{3.14}$$

$$\beta_1(n_f) = \frac{34}{3}C_A^2 - 4\left(\frac{5}{3}C_A + C_F\right)T_F n_f. \tag{3.15}$$

The evolution equation for the renormalized coupling constant is then given by

$$\frac{d a_s(\mu^2)}{d\ln(\mu^2)} = \frac{1}{2}\varepsilon a_s(\mu^2) - \sum_{k=0}^{\infty}\beta_k a_s^{k+2}(\mu^2). \tag{3.16}$$

The factorization relation (2.5) strictly requires that the external massless particles are on shell. Massive loop corrections to the gluon- and ghost-propagators violate this condition, which has to be enforced subtracting the corresponding corrections. They can be uniquely absorbed into the strong coupling constant applying the background field method [52–54]. Here, Z_g can be obtained by only considering the gluon propagator. After mass renormalization in the on-shell scheme via Eq. (3.5), we obtain for the heavy quark contributions to the gluon self-energy

$$\begin{aligned}&\hat{\Pi}^{\mu\nu}_{H,ab,\mathrm{BF}}(p^2, m^2, \mu^2, \varepsilon, \hat{a}_s) = i\left(-p^2 g^{\mu\nu} + p^\mu p^\nu\right)\delta_{ab}\hat{\Pi}_{H,\mathrm{BF}}(p^2, m^2, \mu^2, \varepsilon, \hat{a}_s), \\ &\hat{\Pi}_{H,\mathrm{BF}}(0, m^2, \mu^2, \varepsilon, \hat{a}_s) \\ &\quad = \hat{a}_s \frac{2\beta_{0,Q}}{\varepsilon}\left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2}\exp\left(\sum_{i=2}^{\infty}\frac{\zeta_i}{i}\left(\frac{\varepsilon}{2}\right)^i\right) \\ &\qquad + \hat{a}_s^2\left(\frac{m^2}{\mu^2}\right)^{\varepsilon}\left[\frac{1}{\varepsilon}\left(-\frac{20}{3}T_F C_A - 4T_F C_F\right) - \frac{32}{9}T_F C_A + 15 T_F C_F \right. \\ &\qquad \left. + \varepsilon\left(-\frac{86}{27}T_F C_A - \frac{31}{4}T_F C_F - \frac{5}{3}\zeta_2 T_F C_A - \zeta_2 T_F C_F\right)\right] + O\left(\hat{a}_s^3\right).\end{aligned} \tag{3.17}$$

Note, that although the $O(\hat{a}_s)$-term in the above formula is an expression to all orders in ε, the $O(\hat{a}_s^2)$-term and hence the formula in general only holds up to $O(\varepsilon)$. We have used the Feynman rules of the background field formalism as given in Ref. [55]. In the following, we define

$$f(\varepsilon) \equiv \left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} \exp\left(\sum_{i=2}^{\infty} \frac{\zeta_i}{i}\left(\frac{\varepsilon}{2}\right)^i\right). \tag{3.18}$$

The renormalization constant of the background field Z_A is related to Z_g via

$$Z_A = Z_g^{-2}. \tag{3.19}$$

The light-flavor contributions to Z_A, $Z_{A,l}$, can thus be determined by combining Eqs. (3.11) and (3.19). The heavy flavor part, $Z_{A,H}$, follows from the condition

$$\Pi_{H,\mathrm{BF}}\big(0, \mu^2, a_s, m^2\big) + Z_{A,H} \equiv 0, \tag{3.20}$$

which ensures that the on-shell gluon remains strictly massless. Thus we define the renormalization constant of the strong coupling with n_f light and one heavy flavor as

$$Z_g^{\mathsf{MOM}}(\varepsilon, n_f+1, \mu, m) \equiv \frac{1}{(Z_{A,l} + Z_{A,H})^{1/2}} \tag{3.21}$$

and obtain

$$\begin{aligned} &Z_g^{\mathsf{MOM}^2}(\varepsilon, m, \mu, n_f+1) \\ &\quad = 1 + a_s^{\mathsf{MOM}}\big(\mu^2\big)\left[\frac{2}{\varepsilon}\big(\beta_0(n_f) + \beta_{0,Q} f(\varepsilon)\big)\right] \\ &\qquad + a_s^{\mathsf{MOM}^2}\big(\mu^2\big)\left[\frac{\beta_1(n_f)}{\varepsilon} + \frac{4}{\varepsilon^2}\big(\beta_0(n_f) + \beta_{0,Q} f(\varepsilon)\big)^2\right. \\ &\qquad \left. + \frac{1}{\varepsilon}\left(\frac{m^2}{\mu^2}\right)^{\varepsilon}\big(\beta_{1,Q} + \varepsilon\beta_{1,Q}^{(1)} + \varepsilon^2\beta_{1,Q}^{(2)}\big)\right] + O\big(\varepsilon^2, a_s^{\mathsf{MOM}^3}\big), \end{aligned} \tag{3.22}$$

with

$$\beta_{0,Q} = -\frac{4}{3} T_F, \tag{3.23}$$

$$\beta_{1,Q} = -4\left(\frac{5}{3} C_A + C_F\right) T_F, \tag{3.24}$$

$$\beta_{1,Q}^{(1)} = -\frac{32}{9} T_F C_A + 15 T_F C_F, \tag{3.25}$$

$$\beta_{1,Q}^{(2)} = -\frac{86}{27} T_F C_A - \frac{31}{4} T_F C_F - \zeta_2\left(\frac{5}{3} T_F C_A + T_F C_F\right). \tag{3.26}$$

The coefficients corresponding to Eq. (3.11) expressed in the MOM-scheme read

$$\delta a_{s,1}^{\mathsf{MOM}} = \left[\frac{2\beta_0(n_f)}{\varepsilon} + \frac{2\beta_{0,Q}}{\varepsilon} f(\varepsilon)\right], \tag{3.27}$$

$$\begin{aligned} \delta a_{s,2}^{\mathsf{MOM}} = &\left[\frac{\beta_1(n_f)}{\varepsilon} + \left\{\frac{2\beta_0(n_f)}{\varepsilon} + \frac{2\beta_{0,Q}}{\varepsilon} f(\varepsilon)\right\}^2\right. \\ &\left. + \frac{1}{\varepsilon}\left(\frac{m^2}{\mu^2}\right)^{\varepsilon}\big(\beta_{1,Q} + \varepsilon\beta_{1,Q}^{(1)} + \varepsilon^2\beta_{1,Q}^{(2)}\big)\right] + O\big(\varepsilon^2\big). \end{aligned} \tag{3.28}$$

Since the $\overline{\mathsf{MS}}$-scheme is commonly used, we transform our results back from the MOM-description into the $\overline{\mathsf{MS}}$-scheme, in order to be able to compare to other analyzes. This is achieved by observing that the bare coupling does not change under this transformation and one thus obtains the condition

$$Z_g^{\overline{\mathsf{MS}}^2}(\varepsilon, n_f+1) a_s^{\overline{\mathsf{MS}}}(\mu^2) = Z_g^{\mathsf{MOM}^2}(\varepsilon, m, \mu, n_f+1) a_s^{\mathsf{MOM}}(\mu^2). \tag{3.29}$$

The following relations hold:

$$a_s^{\mathsf{MOM}} = a_s^{\overline{\mathsf{MS}}} - \beta_{0,Q} \ln\left(\frac{m^2}{\mu^2}\right) a_s^{\overline{\mathsf{MS}}^2} + \left[\beta_{0,Q}^2 \ln^2\left(\frac{m^2}{\mu^2}\right) - \beta_{1,Q} \ln\left(\frac{m^2}{\mu^2}\right) - \beta_{1,Q}^{(1)}\right] a_s^{\overline{\mathsf{MS}}^3}, \tag{3.30}$$

or

$$\begin{aligned} a_s^{\overline{\mathsf{MS}}} = {} & a_s^{\mathsf{MOM}} + a_s^{\mathsf{MOM}^2}\left(\delta a_{s,1}^{\mathsf{MOM}} - \delta a_{s,1}^{\overline{\mathsf{MS}}}(n_f+1)\right) + a_s^{\mathsf{MOM}^3}\left(\delta a_{s,2}^{\mathsf{MOM}} - \delta a_{s,2}^{\overline{\mathsf{MS}}}(n_f+1)\right. \\ & \left. - 2\delta a_{s,1}^{\overline{\mathsf{MS}}}(n_f+1)\left[\delta a_{s,1}^{\mathsf{MOM}} - \delta a_{s,1}^{\overline{\mathsf{MS}}}(n_f+1)\right]\right) + O\left(a_s^{\mathsf{MOM}^4}\right), \end{aligned} \tag{3.31}$$

vice versa. Eq. (3.31) is valid to all orders in ε. Here, $a_s^{\overline{\mathsf{MS}}} = a_s^{\overline{\mathsf{MS}}}(n_f+1)$. Applying the on-shell scheme for mass renormalization and the described MOM-scheme for the renormalization of the coupling, one obtains as general formula for mass and coupling constant renormalization up to $O(a_s^{\mathsf{MOM}^3})$

$$\begin{aligned} \hat{A}_{ij} = {} & \delta_{ij} + a_s^{\mathsf{MOM}} \hat{\hat{A}}_{ij}^{(1)} + a_s^{\mathsf{MOM}^2}\left[\hat{\hat{A}}_{ij}^{(2)} + \delta m_1 \left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} m \frac{d}{dm} \hat{\hat{A}}_{ij}^{(1)} + \delta a_{s,1}^{\mathsf{MOM}} \hat{\hat{A}}_{ij}^{(1)}\right] \\ & + a_s^{\mathsf{MOM}^3}\left[\hat{\hat{A}}_{ij}^{(3)} + \delta a_{s,2}^{\mathsf{MOM}} \hat{\hat{A}}_{ij}^{(1)} + 2\delta a_{s,1}^{\mathsf{MOM}}\left(\hat{\hat{A}}_{ij}^{(2)} + \delta m_1\left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} m \frac{d}{dm}\hat{\hat{A}}_{ij}^{(1)}\right)\right. \\ & + \delta m_1 \left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} m \frac{d}{dm} \hat{\hat{A}}_{ij}^{(2)} + \delta m_2 \left(\frac{m^2}{\mu^2}\right)^{\varepsilon} m \frac{d}{dm} \hat{\hat{A}}_{ij}^{(1)} \\ & \left. + \frac{\delta m_1^2}{2}\left(\frac{m^2}{\mu^2}\right)^{\varepsilon} m^2 \frac{d^2}{dm^2} \hat{\hat{A}}_{ij}^{(1)}\right], \end{aligned} \tag{3.32}$$

where we have suppressed the dependence on m, ε and N in the arguments.[6]

3.3. Operator renormalization

The renormalization of the ultra-violet (UV) singularities of the composite operators is done introducing the corresponding Z_{ij}-factors. We consider first the case of n_f massless flavors, cf. [56],

$$A_{qq}^{\mathsf{NS}}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\mathsf{MS}}}, n_f, N\right) = Z_{qq}^{-1,\mathsf{NS}}\left(a_s^{\overline{\mathsf{MS}}}, n_f, \varepsilon, N\right) \hat{A}_{qq}^{\mathsf{NS}}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\mathsf{MS}}}, n_f, \varepsilon, N\right), \tag{3.33}$$

$$\begin{aligned} & A_{ij}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\mathsf{MS}}}, n_f, N\right) = Z_{il}^{-1}\left(a_s^{\overline{\mathsf{MS}}}, n_f, \varepsilon, N\right) \hat{A}_{lj}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\mathsf{MS}}}, n_f, \varepsilon, N\right), \\ & i, j, l = q, g, \end{aligned} \tag{3.34}$$

[6] Here we corrected a typographical error in [34, Eq. (48)].

for the non-singlet and singlet case, with p a space-like momentum. As mentioned before, we neglected all terms being associated to EOM and NGI parts, since they do not contribute in the renormalization of the massive on-shell operator matrix elements. The NS and PS contributions are separated via

$$Z_{qq}^{-1} = Z_{qq}^{-1,\mathrm{PS}} + Z_{qq}^{-1,\mathrm{NS}}, \tag{3.35}$$

$$A_{qq} = A_{qq}^{\mathrm{PS}} + A_{qq}^{\mathrm{NS}}. \tag{3.36}$$

The anomalous dimensions γ_{ij} of the operators are then given by

$$\gamma_{qq}^{\mathrm{NS}}\big(a_s^{\overline{\mathrm{MS}}}, n_f, N\big) = \mu \frac{d}{d\mu} \ln Z_{qq}^{\mathrm{NS}}\big(a_s^{\overline{\mathrm{MS}}}, n_f, \varepsilon, N\big), \tag{3.37}$$

$$\gamma_{ij}\big(a_s^{\overline{\mathrm{MS}}}, n_f, N\big) = Z_{il}^{-1}\big(a_s^{\overline{\mathrm{MS}}}, n_f, \varepsilon, N\big)\mu \frac{d}{d\mu} Z_{lj}\big(a_s^{\overline{\mathrm{MS}}}, n_f, \varepsilon, N\big). \tag{3.38}$$

They can be expanded into a perturbative series as follows

$$\gamma_{ij}^{\mathrm{S,PS,NS}}\big(a_s^{\overline{\mathrm{MS}}}, n_f, N\big) = \sum_{l=1}^{\infty} a_s^{\overline{\mathrm{MS}}^l} \gamma_{ij}^{(l),\mathrm{S,PS,NS}}(n_f, N), \tag{3.39}$$

where the PS contribution starts at $O(a_s^2)$. The anomalous dimensions are known for all N at LO [57,58], and NLO [10–16]. Fixed moments at NNLO have been calculated in Refs. [23–25] and the complete result has been obtained in Refs. [18,19]. At the level of twist-2, they are connected to the splitting functions, [59], by a Mellin-transform[7]

$$\gamma_{ij}^{(k)}(n_f, N) = -\int_0^1 dz\, z^{N-1} P_{ij}^{(k)}(n_f, z). \tag{3.40}$$

In the following, we do not write the dependence on the Mellin-variable N for the OMEs, the operator Z-factors and the anomalous dimensions explicitly. Furthermore, we will suppress the dependence on ε for unrenormalized quantities and Z-factors. From Eqs. (3.37), (3.38), one can determine the relation between the anomalous dimensions and the Z-factors order by order in perturbation theory. In the general case, one finds

$$\begin{aligned} Z_{ij}\big(a_s^{\overline{\mathrm{MS}}}, n_f\big) = {} & \delta_{ij} + a_s^{\overline{\mathrm{MS}}} \frac{\gamma_{ij}^{(0)}}{\varepsilon} + a_s^{\overline{\mathrm{MS}}^2} \left\{ \frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{il}^{(0)}\gamma_{lj}^{(0)} + \beta_0 \gamma_{ij}^{(0)}\right) + \frac{1}{2\varepsilon}\gamma_{ij}^{(1)} \right\} \\ & + a_s^{\overline{\mathrm{MS}}^3} \left\{ \frac{1}{\varepsilon^3}\left(\frac{1}{6}\gamma_{il}^{(0)}\gamma_{lk}^{(0)}\gamma_{kj}^{(0)} + \beta_0 \gamma_{il}^{(0)}\gamma_{lj}^{(0)} + \frac{4}{3}\beta_0^2 \gamma_{ij}^{(0)}\right) \right. \\ & \left. + \frac{1}{\varepsilon^2}\left(\frac{1}{6}\gamma_{il}^{(1)}\gamma_{lj}^{(0)} + \frac{1}{3}\gamma_{il}^{(0)}\gamma_{lj}^{(1)} + \frac{2}{3}\beta_0\gamma_{ij}^{(1)} + \frac{2}{3}\beta_1\gamma_{ij}^{(0)}\right) + \frac{\gamma_{ij}^{(2)}}{3\varepsilon} \right\}. \end{aligned} \tag{3.41}$$

[7] Due to our convention, Eqs. (3.37), (3.38), there is a relative factor of 2 between the anomalous dimensions considered in this work and Refs. [18,19].

The NS and PS Z-factors are given by[8]

$$\begin{aligned}
Z_{qq}^{\mathsf{NS}}\big(a_s^{\overline{\mathsf{MS}}}, n_f, \mu\big) &= 1 + a_s^{\overline{\mathsf{MS}}} \frac{\gamma_{qq}^{(0),\mathsf{NS}}}{\varepsilon} + a_s^{\overline{\mathsf{MS}}^2} \left\{ \frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{qq}^{(0),\mathsf{NS}^2} + \beta_0 \gamma_{qq}^{(0),\mathsf{NS}}\right) + \frac{1}{2\varepsilon}\gamma_{qq}^{(1),\mathsf{NS}} \right\} \\
&\quad + a_s^{\overline{\mathsf{MS}}^3} \left\{ \frac{1}{\varepsilon^3}\left(\frac{1}{6}\gamma_{qq}^{(0),\mathsf{NS}^3} + \beta_0 \gamma_{qq}^{(0),\mathsf{NS}^2} + \frac{4}{3}\beta_0^2 \gamma_{qq}^{(0),\mathsf{NS}}\right) \right. \\
&\quad + \frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{qq}^{(0),\mathsf{NS}}\gamma_{qq}^{(1),\mathsf{NS}} + \frac{2}{3}\beta_0\gamma_{qq}^{(1),\mathsf{NS}} + \frac{2}{3}\beta_1\gamma_{qq}^{(0),\mathsf{NS}}\right) \\
&\quad \left. + \frac{1}{3\varepsilon}\gamma_{qq}^{(2),\mathsf{NS}} \right\}, \qquad (3.42)
\end{aligned}$$

$$\begin{aligned}
Z_{qq}^{\mathsf{PS}}\big(a_s^{\overline{\mathsf{MS}}}, n_f\big) &= a_s^{\overline{\mathsf{MS}}^2} \left\{ \frac{1}{2\varepsilon^2}\gamma_{qg}^{(0)}\gamma_{gq}^{(0)} + \frac{1}{2\varepsilon}\gamma_{qq}^{(1),\mathsf{PS}} \right\} + a_s^{\overline{\mathsf{MS}}^3} \left\{ \frac{1}{\varepsilon^3}\left(\frac{1}{3}\gamma_{qq}^{(0)}\gamma_{qg}^{(0)}\gamma_{gq}^{(0)} \right.\right. \\
&\quad \left. + \frac{1}{6}\gamma_{qg}^{(0)}\gamma_{gg}^{(0)}\gamma_{gq}^{(0)} + \beta_0\gamma_{qg}^{(0)}\gamma_{gq}^{(0)}\right) + \frac{1}{\varepsilon^2}\left(\frac{1}{3}\gamma_{qg}^{(0)}\gamma_{gq}^{(1)} \right. \\
&\quad \left.\left. + \frac{1}{6}\gamma_{qg}^{(1)}\gamma_{gq}^{(0)} + \frac{1}{2}\gamma_{qq}^{(0)}\gamma_{qq}^{(1),\mathsf{PS}} + \frac{2}{3}\beta_0\gamma_{qq}^{(1),\mathsf{PS}}\right) + \frac{\gamma_{qq}^{(2),\mathsf{PS}}}{3\varepsilon} \right\}. \qquad (3.43)
\end{aligned}$$

All quantities in Eqs. (3.41)–(3.43) refer to n_f light flavors and renormalize the massless off-shell OMEs given in Eqs. (3.33), (3.34).

In the next step, we consider an additional heavy quark with mass m. We keep the external momentum artificially off-shell for the moment, in order to deal with the UV-singularities only. For the additional massive quark, one has to account for the prescription of the renormalization of the coupling constant we used in Eqs. (3.27), (3.28). The Z-factors including one massive quark are then obtained by taking Eqs. (3.41)–(3.43) at $n_f + 1$ flavors and performing the scheme transformation given in (3.31). The emergence of $\delta a_{s,k}^{\mathsf{MOM}}$ in Z_{ij} is due to the finite mass effects and cancels singularities which emerge for real radiation and virtual processes at $p^2 \to 0$. Thus one obtains

$$\begin{aligned}
&Z_{ij}^{-1}\big(a_s^{\mathsf{MOM}}, n_f+1, \mu\big) \\
&= \delta_{ij} - a_s^{\mathsf{MOM}}\frac{\gamma_{ij}^{(0)}}{\varepsilon} + a_s^{\mathsf{MOM}^2}\left[\frac{1}{\varepsilon}\left(-\frac{1}{2}\gamma_{ij}^{(1)} - \delta a_{s,1}^{\mathsf{MOM}}\gamma_{ij}^{(0)}\right) + \frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{il}^{(0)}\gamma_{lj}^{(0)} + \beta_0\gamma_{ij}^{(0)}\right)\right] \\
&\quad + a_s^{\mathsf{MOM}^3}\left[\frac{1}{\varepsilon}\left(-\frac{1}{3}\gamma_{ij}^{(2)} - \delta a_{s,1}^{\mathsf{MOM}}\gamma_{ij}^{(1)} - \delta a_{s,2}^{\mathsf{MOM}}\gamma_{ij}^{(0)}\right) \right. \\
&\quad + \frac{1}{\varepsilon^2}\left(\frac{4}{3}\beta_0\gamma_{ij}^{(1)} + 2\delta a_{s,1}^{\mathsf{MOM}}\beta_0\gamma_{ij}^{(0)} + \frac{1}{3}\beta_1\gamma_{ij}^{(0)} + \delta a_{s,1}^{\mathsf{MOM}}\gamma_{il}^{(0)}\gamma_{lj}^{(0)} \right. \\
&\quad \left. + \frac{1}{3}\gamma_{il}^{(1)}\gamma_{lj}^{(0)} + \frac{1}{6}\gamma_{il}^{(0)}\gamma_{lj}^{(1)}\right) \\
&\quad \left. + \frac{1}{\varepsilon^3}\left(-\frac{4}{3}\beta_0^2\gamma_{ij}^{(0)} - \beta_0\gamma_{il}^{(0)}\gamma_{lj}^{(0)} - \frac{1}{6}\gamma_{il}^{(0)}\gamma_{lk}^{(0)}\gamma_{kj}^{(0)}\right)\right], \qquad (3.44)
\end{aligned}$$

[8] In Eq. (3.43) we corrected typographical errors contained in Eq. (34) [34].

and

$$
\begin{aligned}
Z_{qq}^{-1,\mathsf{NS}}\big(a_s^{\mathsf{MOM}}, n_f+1\big) = {} & 1 - a_s^{\mathsf{MOM}}\frac{\gamma_{qq}^{(0),\mathsf{NS}}}{\varepsilon} + a_s^{\mathsf{MOM}^2}\Bigg[\frac{1}{\varepsilon}\left(-\frac{1}{2}\gamma_{qq}^{(1),\mathsf{NS}} - \delta a_{s,1}^{\mathsf{MOM}}\gamma_{qq}^{(0),\mathsf{NS}}\right) \\
& + \frac{1}{\varepsilon^2}\left(\beta_0\gamma_{qq}^{(0),\mathsf{NS}} + \frac{1}{2}\gamma_{qq}^{(0),\mathsf{NS}^2}\right)\Bigg] \\
& + a_s^{\mathsf{MOM}^3}\Bigg[\frac{1}{\varepsilon}\left(-\frac{1}{3}\gamma_{qq}^{(2),\mathsf{NS}} - \delta a_{s,1}^{\mathsf{MOM}}\gamma_{qq}^{(1),\mathsf{NS}} - \delta a_{s,2}^{\mathsf{MOM}}\gamma_{qq}^{(0),\mathsf{NS}}\right) \\
& + \frac{1}{\varepsilon^2}\left(\frac{4}{3}\beta_0\gamma_{qq}^{(1),\mathsf{NS}} + 2\delta a_{s,1}^{\mathsf{MOM}}\beta_0\gamma_{qq}^{(0),\mathsf{NS}} + \frac{1}{3}\beta_1\gamma_{qq}^{(0),\mathsf{NS}} \right.\\
& \left. + \frac{1}{2}\gamma_{qq}^{(0),\mathsf{NS}}\gamma_{qq}^{(1),\mathsf{NS}} + \delta a_{s,1}^{\mathsf{MOM}}\gamma_{qq}^{(0),\mathsf{NS}^2}\right) \\
& + \frac{1}{\varepsilon^3}\left(-\frac{4}{3}\beta_0^2\gamma_{qq}^{(0),\mathsf{NS}} - \beta_0\gamma_{qq}^{(0),\mathsf{NS}^2} - \frac{1}{6}\gamma_{qq}^{(0),\mathsf{NS}^3}\right)\Bigg],
\end{aligned} \tag{3.45}
$$

$$
\begin{aligned}
& Z_{qq}^{-1,\mathsf{PS}}\big(a_s^{\mathsf{MOM}}, n_f+1\big) \\
& \quad = a_s^{\mathsf{MOM}^2}\Bigg[\frac{1}{\varepsilon}\left(-\frac{1}{2}\gamma_{qq}^{(1),\mathsf{PS}}\right) \\
& \qquad + \frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{qg}^{(0)}\gamma_{gq}^{(0)}\right)\Bigg] + a_s^{\mathsf{MOM}^3}\Bigg[\frac{1}{\varepsilon}\left(-\frac{1}{3}\gamma_{qq}^{(2),\mathsf{PS}} - \delta a_{s,1}^{\mathsf{MOM}}\gamma_{qq}^{(1),\mathsf{PS}}\right) \\
& \qquad + \frac{1}{\varepsilon^2}\left(\frac{1}{6}\gamma_{qg}^{(0)}\gamma_{gq}^{(1)} + \frac{1}{3}\gamma_{gq}^{(0)}\gamma_{qg}^{(1)} + \frac{1}{2}\gamma_{qq}^{(0)}\gamma_{qq}^{(1),\mathsf{PS}} + \frac{4}{3}\beta_0\gamma_{qq}^{(1),\mathsf{PS}} + \delta a_{s,1}^{\mathsf{MOM}}\gamma_{qg}^{(0)}\gamma_{gq}^{(0)}\right) \\
& \qquad + \frac{1}{\varepsilon^3}\left(-\frac{1}{3}\gamma_{qg}^{(0)}\gamma_{gq}^{(0)}\gamma_{qq}^{(0)} - \frac{1}{6}\gamma_{gq}^{(0)}\gamma_{qg}^{(0)}\gamma_{gg}^{(0)} - \beta_0\gamma_{qg}^{(0)}\gamma_{gq}^{(0)}\right)\Bigg].
\end{aligned} \tag{3.46}
$$

The above equations are given for n_f+1 flavors. One rederives the expressions for n_f light flavors by setting $(n_f+1) =: n_f$ and $\delta a_s^{\mathsf{MOM}} = \delta a_s^{\overline{\mathsf{MS}}}$. As a next step, we split the OMEs into a part involving only light flavors and the heavy flavor part

$$
\begin{aligned}
& \hat{A}_{ij}\big(p^2, m^2, \mu^2, a_s^{\mathsf{MOM}}, n_f+1\big) \\
& \quad = \hat{A}_{ij}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\mathsf{MS}}}, n_f\right) + \hat{A}_{ij}^{Q}\big(p^2, m^2, \mu^2, a_s^{\mathsf{MOM}}, n_f+1\big).
\end{aligned} \tag{3.47}
$$

In (3.47), (3.48), the light-flavor part depends on $a_s^{\overline{\mathsf{MS}}}$, since the prescription adopted for coupling constant renormalization only applies to the massive part. $\hat{A}_{ij}^{Q}$ denotes any massive OME we consider. The correct UV-renormalization prescription for the massive contribution is obtained by subtracting from Eq. (3.47) the terms applying to the light part only:

$$
\begin{aligned}
& \tilde{\hat{A}}_{ij}^{Q}\big(p^2, m^2, \mu^2, a_s^{\mathsf{MOM}}, n_f+1\big) \\
& \quad = Z_{il}^{-1}\big(a_s^{\mathsf{MOM}}, n_f+1, \mu\big)\hat{A}_{ij}^{Q}\big(p^2, m^2, \mu^2, a_s^{\mathsf{MOM}}, n_f+1\big) \\
& \qquad + Z_{il}^{-1}\big(a_s^{\mathsf{MOM}}, n_f+1, \mu\big)\hat{A}_{ij}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\mathsf{MS}}}, n_f\right) \\
& \qquad - Z_{il}^{-1}\big(a_s^{\overline{\mathsf{MS}}}, n_f, \mu\big)\hat{A}_{ij}\left(\frac{-p^2}{\mu^2}, a_s^{\overline{\mathsf{MS}}}, n_f\right),
\end{aligned} \tag{3.48}
$$

where

$$Z_{ij}^{-1} = \delta_{ij} + \sum_{k=1}^{\infty} a_s^k Z_{ij}^{-1,(k)}. \tag{3.49}$$

In the limit $p^2 = 0$, integrals without a scale vanish within dimensional regularization. Hence for the light-flavor OMEs only the term δ_{ij} remains and one obtains after expanding in a_s

$$\begin{aligned}
&\tilde{\tilde{A}}_{ij}^{Q}\left(\frac{m^2}{\mu^2}, a_s^{\mathsf{MOM}}, n_f + 1\right) \\
&\quad = a_s^{\mathsf{MOM}}\left(\hat{A}_{ij}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(1)}(n_f + 1, \mu) - Z_{ij}^{-1,(1)}(n_f)\right) \\
&\qquad + a_s^{\mathsf{MOM}^2}\left(\hat{A}_{ij}^{(2),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(2)}(n_f + 1, \mu) - Z_{ij}^{-1,(2)}(n_f)\right. \\
&\qquad \left. + Z_{ik}^{-1,(1)}(n_f + 1, \mu)\hat{A}_{kj}^{(1),Q}\left(\frac{m^2}{\mu^2}\right)\right) \\
&\qquad + a_s^{\mathsf{MOM}^3}\left(\hat{A}_{ij}^{(3),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(3)}(n_f + 1, \mu)\right. \\
&\qquad - Z_{ij}^{-1,(3)}(n_f) + Z_{ik}^{-1,(1)}(n_f + 1, \mu)\hat{A}_{kj}^{(2),Q}\left(\frac{m^2}{\mu^2}\right) \\
&\qquad \left. + Z_{ik}^{-1,(2)}(n_f + 1, \mu)\hat{A}_{kj}^{(1),Q}\left(\frac{m^2}{\mu^2}\right)\right).
\end{aligned} \tag{3.50}$$

The Z-factors at $n_f + 1$ flavors refer to Eqs. (3.44)–(3.46), whereas those at n_f flavors correspond to the massless case.

3.4. Mass factorization

Finally, we have to remove the collinear singularities contained in $\tilde{\tilde{A}}_{ij}$, which emerge in the limit $p^2 = 0$. They are absorbed into the parton distribution functions. As a generic renormalization formula, generalizing Eqs. (3.33), (3.34), one finds

$$A_{ij} = Z_{il}^{-1} \hat{A}_{lk} \Gamma_{kj}^{-1}. \tag{3.51}$$

The renormalized operator matrix elements are obtained by

$$A_{ij}^{Q}\left(\frac{m^2}{\mu^2}, a_s^{\mathsf{MOM}}, n_f + 1\right) = \tilde{\tilde{A}}_{il}^{Q}\left(\frac{m^2}{\mu^2}, a_s^{\mathsf{MOM}}, n_f + 1\right)\Gamma_{lj}^{-1}. \tag{3.52}$$

If all quarks were massless, the identity [29]

$$\Gamma_{ij} = Z_{ij}^{-1} \tag{3.53}$$

would hold. However, due to the presence of a heavy quark Q, the transition functions $\Gamma(n_f)$ refer only to massless sub-graphs. Hence the Γ-factors contribute up to $O(a_s^2)$ only and do not involve the special scheme adopted for the renormalization of the coupling. Due to Eq. (3.53), they can be read off from Eqs. (3.41)–(3.43).

The renormalized operator matrix elements are then given by:

$$
\begin{aligned}
&A_{ij}^{Q}\left(\frac{m^2}{\mu^2}, a_s^{\mathsf{MOM}}, n_f+1\right) \\
&= a_s^{\mathsf{MOM}}\left(\hat{A}_{ij}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(1)}(n_f+1) - Z_{ij}^{-1,(1)}(n_f)\right) \\
&\quad + a_s^{\mathsf{MOM}^2}\left(\hat{A}_{ij}^{(2),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(2)}(n_f+1) - Z_{ij}^{-1,(2)}(n_f)\right. \\
&\quad + Z_{ik}^{-1,(1)}(n_f+1)\hat{A}_{kj}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) \\
&\quad \left. + \left[\hat{A}_{il}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{il}^{-1,(1)}(n_f+1) - Z_{il}^{-1,(1)}(n_f)\right]\Gamma_{lj}^{-1,(1)}(n_f)\right) \\
&\quad + a_s^{\mathsf{MOM}^3}\left(\hat{A}_{ij}^{(3),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ij}^{-1,(3)}(n_f+1) - Z_{ij}^{-1,(3)}(n_f)\right. \\
&\quad + Z_{ik}^{-1,(1)}(n_f+1)\hat{A}_{kj}^{(2),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{ik}^{-1,(2)}(n_f+1)\hat{A}_{kj}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) \\
&\quad + \left[\hat{A}_{il}^{(1),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{il}^{-1,(1)}(n_f+1) - Z_{il}^{-1,(1)}(n_f)\right]\Gamma_{lj}^{-1,(2)}(n_f) \\
&\quad + \left[\hat{A}_{il}^{(2),Q}\left(\frac{m^2}{\mu^2}\right) + Z_{il}^{-1,(2)}(n_f+1) - Z_{il}^{-1,(2)}(n_f)\right. \\
&\quad \left.\left. + Z_{ik}^{-1,(1)}(n_f+1)\hat{A}_{kl}^{(1),Q}\left(\frac{m^2}{\mu^2}\right)\right]\Gamma_{lj}^{-1,(1)}(n_f)\right). \qquad (3.54)
\end{aligned}
$$

From (3.54) it is obvious that the renormalization of A_{ij}^{Q} to $O(a_s^3)$ requires the 1-loop terms up to $O(\varepsilon^2)$ and the 2-loop terms up to $O(\varepsilon)$, cf. [29,31,33–35]. Finally, we transform the coupling constant back to the $\overline{\mathsf{MS}}$-scheme by using Eq. (3.30). We do not give the explicit formula here, but present the individual renormalized OMEs after this transformation in the next section as perturbative series in $a_s^{\overline{\mathsf{MS}}}$,

$$
\begin{aligned}
A_{ij}^{Q}\left(\frac{m^2}{\mu^2}, a_s^{\overline{\mathsf{MS}}}, n_f+1\right) &= a_s^{\overline{\mathsf{MS}}} A_{ij}^{Q,(1)}\left(\frac{m^2}{\mu^2}, n_f+1\right) + a_s^{\overline{\mathsf{MS}}^2} A_{ij}^{Q,(2)}\left(\frac{m^2}{\mu^2}, n_f+1\right) \\
&\quad + a_s^{\overline{\mathsf{MS}}^3} A_{ij}^{Q,(3)}\left(\frac{m^2}{\mu^2}, n_f+1\right). \qquad (3.55)
\end{aligned}
$$

4. General structure of the massive operator matrix elements

In the following, we present the unrenormalized and renormalized massive operator matrix elements for the specific flavor channels. The pole terms can all be expressed in terms of known renormalization constants, which provides us with a strong check on our calculation. In particular, we obtain the moments of the complete anomalous dimensions up to $O(a_s^2)$, as well as their T_F-terms at $O(a_s^3)$. The moments of the $O(\varepsilon^0)$-terms of the unrenormalized OMEs at the 3-loop level, $a_{ij}^{(3)}$, are a new result. Previously, the $O(\varepsilon)$ terms at the 2-loop level, $\bar{a}_{ij}^{(2)}$, for general values of N were calculated by the present authors in Refs. [34,35]. The pole terms and the

$O(\varepsilon^0)$ terms, $a_{ij}^{(2)}$, at the 2-loop level have been calculated for the first time in Refs. [29,31]. They were confirmed in [33,35], as well as by the present calculation, in which they appear in the renormalization of the respective moments of the 3-loop OMEs. In order to keep up with the notation used in [29,31], we define the 2-loop terms $a_{ij}^{(2)}, \bar{a}_{ij}^{(2)}$ after performing mass renormalization in the on-shell scheme. This we do not apply for the 3-loop terms. We choose to calculate one-particle reducible diagrams and therefore have to include external self-energies containing massive quarks into our calculation. Before presenting the operator matrix elements up to three loops, we first summarize the necessary self-energy contributions.

4.1. Self-energy contributions

The gluon and quark self-energy contributions due to heavy quark lines are given by

$$\hat{\Pi}_{\mu\nu}^{ab}(p^2, \hat{m}^2, \mu^2, \hat{a}_s) = i\delta^{ab}[-g_{\mu\nu}p^2 + p_\mu p_\nu]\hat{\Pi}(p^2, \hat{m}^2, \mu^2, \hat{a}_s), \tag{4.1}$$

with

$$\hat{\Pi}(p^2, \hat{m}^2, \mu^2, \hat{a}_s) = \sum_{k=1}^{\infty} \hat{a}_s^k \hat{\Pi}^{(k)}(p^2, \hat{m}^2, \mu^2) \tag{4.2}$$

and

$$\hat{\Sigma}_{ij}(p^2, \hat{m}^2, \mu^2, \hat{a}_s) = i\delta_{ij}\not{p}\hat{\Sigma}(p^2, \hat{m}^2, \mu^2, \hat{a}_s), \tag{4.3}$$

where

$$\hat{\Sigma}(p^2, \hat{m}^2, \mu^2, \hat{a}_s) = \sum_{k=2}^{\infty} \hat{a}_s^k \hat{\Sigma}^{(k)}(p^2, \hat{m}^2, \mu^2). \tag{4.4}$$

Note, that the quark self-energy contributions start at 2-loop order. These self-energies are easily calculated using MATAD, [60], cf. Section 5. The expansion coefficients for $p^2 = 0$ of Eqs. (4.2), (4.4) are needed for the calculation of the gluonic and quarkonic OMEs. The contributions to the gluon vacuum polarization for general gauge parameter ξ are

$$\hat{\Pi}^{(1)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) = T_F\left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2}\left(-\frac{8}{3\varepsilon}\exp\left(\sum_{i=2}^{\infty}\frac{\zeta_i}{i}\left(\frac{\varepsilon}{2}\right)^i\right)\right), \tag{4.5}$$

$$\begin{aligned}\hat{\Pi}^{(2)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) = T_F\left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\Bigg(&-\frac{4}{\varepsilon^2}C_A + \frac{1}{\varepsilon}\{-12C_F + 5C_A\} + C_A\left(\frac{13}{12} - \zeta_2\right) - \frac{13}{3}C_F \\ &+ \varepsilon\left\{C_A\left(\frac{169}{144} + \frac{5}{4}\zeta_2 - \frac{\zeta_3}{3}\right) + C_F\left(-\frac{35}{12} - 3\zeta_2\right)\right\}\Bigg) + O(\varepsilon^2),\end{aligned} \tag{4.6}$$

$$\begin{aligned}&\hat{\Pi}^{(3)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) \\ &\quad = T_F\left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\left(\frac{1}{\varepsilon^3}\left\{-\frac{32}{9}T_F C_A(2n_f + 1) + C_A^2\left(\frac{164}{9} + \frac{4}{3}\xi\right)\right\}\right. \\ &\qquad + \frac{1}{\varepsilon^2}\left\{\frac{80}{27}(C_A - 6C_F)n_f T_F + \frac{8}{27}(35C_A - 48C_F)T_F\right. \\ &\qquad \left. + \frac{C_A^2}{27}(-781 + 63\xi) + \frac{712}{9}C_A C_F\right\}\end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{\varepsilon}\left\{\frac{4}{27}\big(C_A(-101-18\zeta_2)-62C_F\big)n_fT_F+\frac{2}{27}\big(C_A(-37-18\zeta_2)-80C_F\big)T_F\right.\\
&+C_A^2\left(-12\zeta_3+\frac{41}{6}\zeta_2+\frac{3181}{108}+\frac{\zeta_2}{2}\xi+\frac{137}{36}\xi\right)\\
&\left.+C_AC_F\left(16\zeta_3-\frac{1570}{27}\right)+\frac{272}{3}C_F^2\right\}+n_fT_F\left\{C_A\left(\frac{56}{9}\zeta_3+\frac{10}{9}\zeta_2-\frac{3203}{243}\right)\right.\\
&\left.+C_F\left(-\frac{20}{3}\zeta_2-\frac{1942}{81}\right)\right\}+T_F\left\{C_A\left(-\frac{295}{18}\zeta_3+\frac{35}{9}\zeta_2+\frac{6361}{486}\right)\right.\\
&\left.+C_F\left(-7\zeta_3-\frac{16}{3}\zeta_2-\frac{218}{81}\right)\right\}+C_A^2\left\{4\mathsf{B}_4-27\zeta_4+\frac{1969}{72}\zeta_3-\frac{781}{72}\zeta_2+\frac{42\,799}{3888}\right.\\
&\left.-\frac{7}{6}\zeta_3\xi+\frac{7}{8}\zeta_2\xi+\frac{3577}{432}\xi\right\}+C_AC_F\left\{-8\mathsf{B}_4+36\zeta_4-\frac{1957}{12}\zeta_3+\frac{89}{3}\zeta_2+\frac{10\,633}{81}\right\}\\
&\left.+C_F^2\left\{\frac{95}{3}\zeta_3+\frac{274}{9}\right\}\right)+O(\varepsilon),
\end{aligned}
\tag{4.7}
$$

and for the quark self-energy,

$$
\hat{\Sigma}^{(2)}\left(0,\frac{\hat{m}^2}{\mu^2}\right)=T_FC_F\left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\left\{\frac{2}{\varepsilon}+\frac{5}{6}+\left[\frac{89}{72}+\frac{\zeta_2}{2}\right]\varepsilon\right\}+O\big(\varepsilon^2\big),
\tag{4.8}
$$

$$
\begin{aligned}
\hat{\Sigma}^{(3)}\left(0,\frac{\hat{m}^2}{\mu^2}\right)=T_FC_F\left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}&\left(\frac{8}{3\varepsilon^3}C_A\{1-\xi\}\right.\\
&+\frac{1}{\varepsilon^2}\left\{+\frac{32}{9}T_F(n_f+2)-C_A\left(\frac{40}{9}+4\xi\right)-\frac{8}{3}C_F\right\}\\
&+\frac{1}{\varepsilon}\left\{\frac{40}{27}T_F(n_f+2)+C_A\left\{\zeta_2+\frac{454}{27}-\zeta_2\xi-\frac{70}{9}\xi\right\}-26C_F\right\}\\
&+n_fT_F\left\{\frac{4}{3}\zeta_2+\frac{674}{81}\right\}+T_F\left\{\frac{8}{3}\zeta_2+\frac{604}{81}\right\}\\
&+C_A\left\{\frac{17}{3}\zeta_3-\frac{5}{3}\zeta_2+\frac{1879}{162}+\frac{7}{3}\zeta_3\xi-\frac{3}{2}\zeta_2\xi-\frac{407}{27}\xi\right\}\\
&\left.+C_F\left\{-8\zeta_3-\zeta_2-\frac{335}{18}\right\}\right)+O(\varepsilon),
\end{aligned}
\tag{4.9}
$$

see also [40,61]. In Eq. (4.7) the constant

$$
\begin{aligned}
\mathsf{B}_4&=-4\zeta_2\ln^2(2)+\frac{2}{3}\ln^4(2)-\frac{13}{2}\zeta_4+16\mathrm{Li}_4\left(\frac{1}{2}\right)\\
&\approx-1.762800093\ldots
\end{aligned}
\tag{4.10}
$$

appears.

4.2. $A_{qq,Q}^{\mathsf{NS}}$

The lowest NS-contribution is of $O(a_s^2)$,

$$
A_{qq,Q}^{\mathsf{NS}}=a_s^2A_{qq,Q}^{(2),\mathsf{NS}}+a_s^3A_{qq,Q}^{(3),\mathsf{NS}}+O\big(a_s^4\big).
\tag{4.11}
$$

The expansion coefficients are obtained in the MOM-scheme from the bare quantities, using Eqs. (3.32), (3.54). After operator renormalization and mass factorization, the OMEs are given by

$$A_{qq,Q}^{(2),\mathsf{NS},\mathsf{MOM}} = \hat{A}_{qq,Q}^{(2),\mathsf{NS},\mathsf{MOM}} + Z_{qq}^{-1,(2),\mathsf{NS}}(n_f+1) - Z_{qq}^{-1,(2),\mathsf{NS}}(n_f), \tag{4.12}$$

$$\begin{aligned} A_{qq,Q}^{(3),\mathsf{NS},\mathsf{MOM}} &= \hat{A}_{qq,Q}^{(3),\mathsf{NS},\mathsf{MOM}} + Z_{qq}^{-1,(3),\mathsf{NS}}(n_f+1) - Z_{qq}^{-1,(3),\mathsf{NS}}(n_f) \\ &\quad + Z_{qq}^{-1,(1),\mathsf{NS}}(n_f+1)\hat{A}_{qq,Q}^{(2),\mathsf{NS},\mathsf{MOM}} \\ &\quad + \big[\hat{A}_{qq,Q}^{(2),\mathsf{NS},\mathsf{MOM}} + Z_{qq}^{-1,(2),\mathsf{NS}}(n_f+1) - Z_{qq}^{-1,(2),\mathsf{NS}}(n_f)\big]\Gamma_{qq}^{-1,(1)}(n_f). \end{aligned} \tag{4.13}$$

From (3.32), (3.54), (4.12), (4.13), one predicts the pole terms of the unrenormalized OME. At second and third order they read

$$\hat{\hat{A}}_{qq,Q}^{(2),\mathsf{NS}} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\left(\frac{\beta_{0,Q}\gamma_{qq}^{(0)}}{\varepsilon^2} + \frac{\hat{\gamma}_{qq}^{(1),\mathsf{NS}}}{2\varepsilon} + a_{qq,Q}^{(2),\mathsf{NS}} + \bar{a}_{qq,Q}^{(2),\mathsf{NS}}\varepsilon\right), \tag{4.14}$$

$$\begin{aligned} \hat{\hat{A}}_{qq,Q}^{(3),\mathsf{NS}} &= \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}\left\{-\frac{4\gamma_{qq}^{(0)}\beta_{0,Q}}{3\varepsilon^3}(\beta_0+2\beta_{0,Q})\right. \\ &\quad + \frac{1}{\varepsilon^2}\left(\frac{2\gamma_{qq}^{(1),\mathsf{NS}}\beta_{0,Q}}{3} - \frac{4\hat{\gamma}_{qq}^{(1),\mathsf{NS}}}{3}[\beta_0+\beta_{0,Q}] + \frac{2\beta_{1,Q}\gamma_{qq}^{(0)}}{3} - 2\delta m_1^{(-1)}\beta_{0,Q}\gamma_{qq}^{(0)}\right) \\ &\quad + \frac{1}{\varepsilon}\left(\frac{\hat{\gamma}_{qq}^{(2),\mathsf{NS}}}{3} - 4a_{qq,Q}^{(2),\mathsf{NS}}[\beta_0+\beta_{0,Q}] + \beta_{1,Q}^{(1)}\gamma_{qq}^{(0)}\right. \\ &\quad \left.\left. + \frac{\gamma_{qq}^{(0)}\beta_0\beta_{0,Q}\zeta_2}{2} - 2\delta m_1^{(0)}\beta_{0,Q}\gamma_{qq}^{(0)} - \delta m_1^{(-1)}\hat{\gamma}_{qq}^{(1),\mathsf{NS}}\right) + a_{qq,Q}^{(3),\mathsf{NS}}\right\}. \end{aligned} \tag{4.15}$$

Note, that we have already used the general structure of the unrenormalized lower order OME in the evaluation of the $O(\hat{a}_s^3)$ term, as we will always do in the following. Using Eqs. (4.12), (4.13), (3.32), one can renormalize the above expressions. In addition, we finally transform back to the $\overline{\mathsf{MS}}$-scheme using Eq. (3.30). Thus one obtains the renormalized expansion coefficients of Eq. (4.11)

$$A_{qq,Q}^{(2),\mathsf{NS},\overline{\mathsf{MS}}} = \frac{\beta_{0,Q}\gamma_{qq}^{(0)}}{4}\ln^2\left(\frac{m^2}{\mu^2}\right) + \frac{\hat{\gamma}_{qq}^{(1),\mathsf{NS}}}{2}\ln\left(\frac{m^2}{\mu^2}\right) + a_{qq,Q}^{(2),\mathsf{NS}} - \frac{\beta_{0,Q}\gamma_{qq}^{(0)}}{4}\zeta_2, \tag{4.16}$$

$$\begin{aligned} A_{qq,Q}^{(3),\mathsf{NS},\overline{\mathsf{MS}}} &= -\frac{\gamma_{qq}^{(0)}\beta_{0,Q}}{6}(\beta_0+2\beta_{0,Q})\ln^3\left(\frac{m^2}{\mu^2}\right) \\ &\quad + \frac{1}{4}\left\{2\gamma_{qq}^{(1),\mathsf{NS}}\beta_{0,Q} - 2\hat{\gamma}_{qq}^{(1),\mathsf{NS}}(\beta_0+\beta_{0,Q}) + \beta_{1,Q}\gamma_{qq}^{(0)}\right\}\ln^2\left(\frac{m^2}{\mu^2}\right) \\ &\quad + \frac{1}{2}\left\{\hat{\gamma}_{qq}^{(2),\mathsf{NS}} - \left(4a_{qq,Q}^{(2),\mathsf{NS}} - \zeta_2\beta_{0,Q}\gamma_{qq}^{(0)}\right)(\beta_0+\beta_{0,Q}) + \gamma_{qq}^{(0)}\beta_{1,Q}^{(1)}\right\}\ln\left(\frac{m^2}{\mu^2}\right) \\ &\quad + 4\bar{a}_{qq,Q}^{(2),\mathsf{NS}}(\beta_0+\beta_{0,Q}) - \gamma_{qq}^{(0)}\beta_{1,Q}^{(2)} - \frac{\gamma_{qq}^{(0)}\beta_0\beta_{0,Q}\zeta_3}{6} - \frac{\gamma_{qq}^{(1),\mathsf{NS}}\beta_{0,Q}\zeta_2}{4} \\ &\quad + 2\delta m_1^{(1)}\beta_{0,Q}\gamma_{qq}^{(0)} + \delta m_1^{(0)}\hat{\gamma}_{qq}^{(1),\mathsf{NS}} + 2\delta m_1^{(-1)}a_{qq,Q}^{(2),\mathsf{NS}} + a_{qq,Q}^{(3),\mathsf{NS}}. \end{aligned} \tag{4.17}$$

Note that in the NS-case, one is generically provided with even and odd moments due to a Ward-identity relating the results in the polarized and unpolarized case. The former refer to the anomalous dimensions $\gamma_{qq}^{\mathsf{NS},+}$ and the latter to $\gamma_{qq}^{\mathsf{NS},-}$ as given in Eqs. (3.5), (3.7) and Eqs. (3.6), (3.8) in Ref. [18]. The relations above also apply to other twist-2 non-singlet massive OMEs, as to transversity, for which the 2- and 3-loop heavy flavor corrections are given in [62].

4.3. A_{Qq}^{PS} and $A_{qq,Q}^{\mathsf{PS}}$

There are two different PS-contributions. The term referring to the case in which the operator couples to a heavy quark, A_{Qq}^{PS}, starts at $O(a_s^2)$, whereas the term in which it couples to an internal light quark line, $A_{qq,Q}^{\mathsf{PS}}$, emerges for the first time at $O(a_s^3)$,

$$A_{Qq}^{\mathsf{PS}} = a_s^2 A_{Qq}^{(2),\mathsf{PS}} + a_s^3 A_{Qq}^{(3),\mathsf{PS}} + O\big(a_s^4\big), \tag{4.18}$$

$$A_{qq,Q}^{\mathsf{PS}} = a_s^3 A_{qq,Q}^{(3),\mathsf{PS}} + O\big(a_s^4\big). \tag{4.19}$$

Separating these contributions is not straightforward, since the generic renormalization formula for operator renormalization and mass factorization, Eq. (3.54), applies to the sum of these terms only. At $O(a_s^2)$, this problem does not occur and renormalization proceeds in the MOM-scheme via

$$\begin{aligned} A_{Qq}^{(2),\mathsf{PS},\mathsf{MOM}} = {} & \hat{A}_{Qq}^{(2),\mathsf{PS},\mathsf{MOM}} + Z_{qq}^{-1,(2),\mathsf{PS}}(n_f+1) - Z_{qq}^{-1,(2),\mathsf{PS}}(n_f) \\ & + \big[\hat{A}_{Qg}^{(1),\mathsf{MOM}} + Z_{qg}^{-1,(1)}(n_f+1) - Z_{qg}^{-1,(1)}(n_f)\big]\Gamma_{gq}^{-1,(1)}(n_f). \end{aligned} \tag{4.20}$$

Thus the unrenormalized expression is given by

$$\hat{\hat{A}}_{Qq}^{(2),\mathsf{PS}} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\left(-\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{2\varepsilon^2} + \frac{\hat{\gamma}_{qq}^{(1),\mathsf{PS}}}{2\varepsilon} + a_{Qq}^{(2),\mathsf{PS}} + \bar{a}_{Qq}^{(2),\mathsf{PS}}\varepsilon\right). \tag{4.21}$$

The renormalized result in the $\overline{\mathsf{MS}}$-scheme reads

$$A_{Qq}^{(2),\mathsf{PS},\overline{\mathsf{MS}}} = -\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{8}\ln^2\left(\frac{m^2}{\mu^2}\right) + \frac{\hat{\gamma}_{qq}^{(1),\mathsf{PS}}}{2}\ln\left(\frac{m^2}{\mu^2}\right) + a_{Qq}^{(2),\mathsf{PS}} + \frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{8}\zeta_2. \tag{4.22}$$

The corresponding renormalization relation at third order is given by

$$\begin{aligned} & A_{Qq}^{(3),\mathsf{PS},\mathsf{MOM}} + A_{qq,Q}^{(2),\mathsf{PS},\mathsf{MOM}} \\ & \quad = \hat{A}_{Qq}^{(3),\mathsf{PS},\mathsf{MOM}} + \hat{A}_{qq,Q}^{(3),\mathsf{PS},\mathsf{MOM}} + Z_{qq}^{-1,(3),\mathsf{PS}}(n_f+1) - Z_{qq}^{-1,(3),\mathsf{PS}}(n_f) \\ & \qquad + Z_{qq}^{-1,(1)}(n_f+1)\hat{A}_{Qq}^{(2),\mathsf{PS},\mathsf{MOM}} + Z_{qg}^{-1,(1)}(n_f+1)\hat{A}_{gq,Q}^{(2),\mathsf{MOM}} \\ & \qquad + \big[\hat{A}_{Qg}^{(1),\mathsf{MOM}} + Z_{qg}^{-1,(1)}(n_f+1) - Z_{qg}^{-1,(1)}(n_f)\big]\Gamma_{gq}^{-1,(2)}(n_f) \\ & \qquad + \big[\hat{A}_{Qq}^{(2),\mathsf{PS},\mathsf{MOM}} + Z_{qq}^{-1,(2),\mathsf{PS}}(n_f+1) - Z_{qq}^{-1,(2),\mathsf{PS}}(n_f)\big]\Gamma_{qq}^{-1,(1)}(n_f) \\ & \qquad + \big[\hat{A}_{Qg}^{(2),\mathsf{MOM}} + Z_{qg}^{-1,(2)}(n_f+1) - Z_{qg}^{-1,(2)}(n_f) \\ & \qquad + Z_{qq}^{-1,(1)}(n_f+1)A_{Qg}^{(1),\mathsf{MOM}} + Z_{qg}^{-1,(1)}(n_f+1)A_{gg,Q}^{(1),\mathsf{MOM}}\big]\Gamma_{gq}^{-1,(1)}(n_f). \end{aligned} \tag{4.23}$$

Taking into account the kinematic and UV-structure of the contributing Feynman diagrams, the two contributions can be separated. For the bare quantities we obtain

$$\begin{aligned}\hat{\hat{A}}_{Qq}^{(3),\mathsf{PS}} = {} & \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}\Bigg[\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{6\varepsilon^3}\left(\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0+16\beta_{0,Q}\right) \\ & + \frac{1}{\varepsilon^2}\Bigg(-\frac{4\hat{\gamma}_{qq}^{(1),\mathsf{PS}}}{3}[\beta_0+\beta_{0,Q}]-\frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(1)}}{3} \\ & + \frac{\hat{\gamma}_{qg}^{(0)}}{6}\left[2\hat{\gamma}_{gq}^{(1)}-\gamma_{gq}^{(1)}\right]+\delta m_1^{(-1)}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}\Bigg)+\frac{1}{\varepsilon}\Bigg(\frac{\hat{\gamma}_{qq}^{(2),\mathsf{PS}}}{3}-n_f\frac{\hat{\tilde{\gamma}}_{qq}^{(2),\mathsf{PS}}}{3} \\ & + \hat{\gamma}_{qg}^{(0)}a_{gq,Q}^{(2)}-\gamma_{gq}^{(0)}a_{Qg}^{(2)}-4(\beta_0+\beta_{0,Q})a_{Qq}^{(2),\mathsf{PS}} \\ & - \frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}\zeta_2}{16}\left[\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0\right] \\ & + \delta m_1^{(0)}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}-\delta m_1^{(-1)}\hat{\gamma}_{qq}^{(1),\mathsf{PS}}\Bigg)+a_{Qq}^{(3),\mathsf{PS}}\Bigg],\end{aligned} \tag{4.24}$$

$$\begin{aligned}\hat{\hat{A}}_{qq,Q}^{(3),\mathsf{PS}} = {} & n_f\left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}\Bigg[\frac{2\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}\beta_{0,Q}}{3\varepsilon^3}+\frac{1}{3\varepsilon^2}\left(2\hat{\gamma}_{qq}^{(1),\mathsf{PS}}\beta_{0,Q}+\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{gq}^{(1)}\right) \\ & + \frac{1}{\varepsilon}\Bigg(\frac{\hat{\tilde{\gamma}}_{qq}^{(2),\mathsf{PS}}}{3}+\hat{\gamma}_{qg}^{(0)}a_{gq,Q}^{(2)}-\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}\beta_{0,Q}\zeta_2}{4}\Bigg)+\frac{a_{qq,Q}^{(3),\mathsf{PS}}}{n_f}\Bigg].\end{aligned} \tag{4.25}$$

The renormalized terms are given in the $\overline{\mathsf{MS}}$-scheme by

$$\begin{aligned}A_{Qq}^{(3),\mathsf{PS},\overline{\mathsf{MS}}} = {} & \frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{48}\left\{\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0+16\beta_{0,Q}\right\}\ln^3\left(\frac{m^2}{\mu^2}\right) \\ & + \frac{1}{8}\left\{-4\hat{\gamma}_{qq}^{(1),\mathsf{PS}}(\beta_0+\beta_{0,Q})+\hat{\gamma}_{qg}^{(0)}\left(\hat{\gamma}_{gq}^{(1)}-\gamma_{gq}^{(1)}\right)-\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(1)}\right\}\ln^2\left(\frac{m^2}{\mu^2}\right) \\ & + \frac{1}{16}\Big\{8\hat{\gamma}_{qq}^{(2),\mathsf{PS}}-8n_f\hat{\tilde{\gamma}}_{qq}^{(2),\mathsf{PS}}-32a_{Qq}^{(2),\mathsf{PS}}(\beta_0+\beta_{0,Q})+8\hat{\gamma}_{qg}^{(0)}a_{gq,Q}^{(2)} \\ & - 8\gamma_{gq}^{(0)}a_{Qg}^{(2)}-\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}\zeta_2\left(\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0+8\beta_{0,Q}\right)\Big\}\ln\left(\frac{m^2}{\mu^2}\right) \\ & + 4(\beta_0+\beta_{0,Q})\bar{a}_{Qq}^{(2),\mathsf{PS}}+\gamma_{gq}^{(0)}\bar{a}_{Qg}^{(2)}-\hat{\gamma}_{qg}^{(0)}\bar{a}_{gq,Q}^{(2)} \\ & + \frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\zeta_3}{48}\left(\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0\right)+\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(1)}\zeta_2}{16} \\ & - \delta m_1^{(1)}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}+\delta m_1^{(0)}\hat{\gamma}_{qq}^{(1),\mathsf{PS}}+2\delta m_1^{(-1)}a_{Qq}^{(2),\mathsf{PS}}+a_{Qq}^{(3),\mathsf{PS}},\end{aligned} \tag{4.26}$$

$$\begin{aligned}A_{qq,Q}^{(3),\mathsf{PS},\overline{\mathsf{MS}}} = {} & n_f\Bigg\{\frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\beta_{0,Q}}{12}\ln^3\left(\frac{m^2}{\mu^2}\right)+\frac{1}{8}\left(4\hat{\gamma}_{qq}^{(1),\mathsf{PS}}\beta_{0,Q}+\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{gq}^{(1)}\right)\ln^2\left(\frac{m^2}{\mu^2}\right) \\ & + \frac{1}{4}\left(2\hat{\tilde{\gamma}}_{qq}^{(2),\mathsf{PS}}+\hat{\gamma}_{qg}^{(0)}\left\{2a_{gq,Q}^{(2)}-\gamma_{gq}^{(0)}\beta_{0,Q}\zeta_2\right\}\right)\ln\left(\frac{m^2}{\mu^2}\right) \\ & - \hat{\gamma}_{qg}^{(0)}\bar{a}_{gq,Q}^{(2)}+\frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\beta_{0,Q}\zeta_3}{12}-\frac{\hat{\gamma}_{qq}^{(1),\mathsf{PS}}\beta_{0,Q}\zeta_2}{4}\Bigg\}+a_{qq,Q}^{(3),\mathsf{PS}}.\end{aligned} \tag{4.27}$$

4.4. A_{Qg} and $A_{qg,Q}$

The OME A_{Qg} is the most complex expression. As in the PS-case, there are two different contributions, depending on whether the operator couples to a light quark line, denoted by $A_{qg,Q}$, or to a heavy quark line, given by A_{Qg},

$$A_{Qg} = a_s A_{Qg}^{(1)} + a_s^2 A_{Qg}^{(2)} + a_s^3 A_{Qg}^{(3)} + O\left(a_s^4\right), \tag{4.28}$$

$$A_{qg,Q} = a_s^3 A_{qg,Q}^{(3)} + O\left(a_s^4\right). \tag{4.29}$$

In the MOM-scheme the 1- and 2-loop contributions obey the following relations

$$A_{Qg}^{(1),\mathsf{MOM}} = \hat{A}_{Qg}^{(1),\mathsf{MOM}} + Z_{qg}^{-1,(1)}(n_f+1) - Z_{qg}^{-1,(1)}(n_f), \tag{4.30}$$

$$\begin{aligned} A_{Qg}^{(2),\mathsf{MOM}} = {} & \hat{A}_{Qg}^{(2),\mathsf{MOM}} + Z_{qg}^{-1,(2)}(n_f+1) - Z_{qg}^{-1,(2)}(n_f) + Z_{qg}^{-1,(1)}(n_f+1)\hat{A}_{gg,Q}^{(1),\mathsf{MOM}} \\ & + Z_{qq}^{-1,(1)}(n_f+1)\hat{A}_{Qg}^{(1),\mathsf{MOM}} + \left[\hat{A}_{Qg}^{(1),\mathsf{MOM}} + Z_{qg}^{-1,(1)}(n_f+1) \right. \\ & \left. - Z_{qg}^{-1,(1)}(n_f)\right]\Gamma_{gg}^{-1,(1)}(n_f). \end{aligned} \tag{4.31}$$

The unrenormalized terms are given by

$$\hat{\hat{A}}_{Qg}^{(1)} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2} \frac{\hat{\gamma}_{qg}^{(0)}}{\varepsilon} \exp\left(\sum_{i=2}^{\infty} \frac{\zeta_i}{i}\left(\frac{\varepsilon}{2}\right)^i\right), \tag{4.32}$$

$$\begin{aligned} \hat{\hat{A}}_{Qg}^{(2)} = {} & \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\left[-\frac{\hat{\gamma}_{qg}^{(0)}}{2\varepsilon^2}\left(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0 + 4\beta_{0,Q}\right) \right. \\ & + \frac{\hat{\gamma}_{qg}^{(1)} - 2\delta m_1^{(-1)}\hat{\gamma}_{qg}^{(0)}}{2\varepsilon} + a_{Qg}^{(2)} - \delta m_1^{(0)}\hat{\gamma}_{qg}^{(0)} \\ & \left. - \frac{\hat{\gamma}_{qg}^{(0)}\beta_{0,Q}\zeta_2}{2} + \varepsilon\left(\bar{a}_{Qg}^{(2)} - \delta m_1^{(1)}\hat{\gamma}_{qg}^{(0)} - \frac{\hat{\gamma}_{qg}^{(0)}\beta_{0,Q}\zeta_2}{12}\right)\right]. \end{aligned} \tag{4.33}$$

Note that we have already made the one-particle reducible contributions to Eq. (4.33) explicit, which are given by the 1-loop contribution multiplied by the 1-loop term of the gluon-self energy, cf. Eq. (4.5). Furthermore, Eq. (4.33) already contains terms which result from mass renormalization in the $O(\varepsilon^0)$ and $O(\varepsilon)$ expressions. At this stage of the renormalization procedure, they should not be present, however, we have included them here in order to have the same notation as in Refs. [29,31] at the 2-loop level. The renormalized terms then become in the $\overline{\mathsf{MS}}$-scheme

$$A_{Qg}^{(1),\overline{\mathsf{MS}}} = \frac{\hat{\gamma}_{qg}^{(0)}}{2}\ln\left(\frac{m^2}{\mu^2}\right), \tag{4.34}$$

$$\begin{aligned} A_{Qg}^{(2),\overline{\mathsf{MS}}} = {} & -\frac{\hat{\gamma}_{qg}^{(0)}}{8}\left[\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0 + 4\beta_{0,Q}\right]\ln^2\left(\frac{m^2}{\mu^2}\right) + \frac{\hat{\gamma}_{qg}^{(1)}}{2}\ln\left(\frac{m^2}{\mu^2}\right) \\ & + a_{Qg}^{(2)} + \frac{\hat{\gamma}_{qg}^{(0)}\zeta_2}{8}\left(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0\right). \end{aligned} \tag{4.35}$$

The generic renormalization relation at the 3-loop level is given by

$$\begin{aligned} & A_{Qg}^{(3),\mathsf{MOM}} + A_{qg,Q}^{(3),\mathsf{MOM}} \\ & \quad = \hat{A}_{Qg}^{(3),\mathsf{MOM}} + \hat{A}_{qg,Q}^{(3),\mathsf{MOM}} + Z_{qg}^{-1,(3)}(n_f+1) - Z_{qg}^{-1,(3)}(n_f) \end{aligned}$$

$$
\begin{aligned}
&+ Z_{qg}^{-1,(2)}(n_f+1)\hat{A}_{gg,Q}^{(1),\mathsf{MOM}} + Z_{qg}^{-1,(1)}(n_f+1)\hat{A}_{gg,Q}^{(2),\mathsf{MOM}} + Z_{qq}^{-1,(2)}(n_f+1)\hat{A}_{Qg}^{(1),\mathsf{MOM}} \\
&+ Z_{qq}^{-1,(1)}(n_f+1)\hat{A}_{Qg}^{(2),\mathsf{MOM}} \\
&+ \big[\hat{A}_{Qg}^{(1),\mathsf{MOM}} + Z_{qg}^{-1,(1)}(n_f+1) - Z_{qg}^{-1,(1)}(n_f)\big]\Gamma_{gg}^{-1,(2)}(n_f) \\
&+ \big[\hat{A}_{Qg}^{(2),\mathsf{MOM}} + Z_{qg}^{-1,(2)}(n_f+1) - Z_{qg}^{-1,(2)}(n_f) + Z_{qq}^{-1,(1)}(n_f+1)A_{Qg}^{(1),\mathsf{MOM}} \\
&+ Z_{qg}^{-1,(1)}(n_f+1)A_{gg,Q}^{(1),\mathsf{MOM}}\big]\Gamma_{gg}^{-1,(1)}(n_f) + \big[\hat{A}_{Qq}^{(2),\mathsf{PS},\mathsf{MOM}} + Z_{qq}^{-1,(2),\mathsf{PS}}(n_f+1) \\
&- Z_{qq}^{-1,(2),\mathsf{PS}}(n_f)\big]\Gamma_{qg}^{-1,(1)}(n_f) + \big[\hat{A}_{qq,Q}^{(2),\mathsf{NS},\mathsf{MOM}} + Z_{qq}^{-1,(2),\mathsf{NS}}(n_f+1) \\
&- Z_{qq}^{-1,(2),\mathsf{NS}}(n_f)\big]\Gamma_{qg}^{-1,(1)}(n_f). \qquad (4.36)
\end{aligned}
$$

Similar to the PS-case, the different contributions can be separated and one obtains the following unrenormalized results

$$
\begin{aligned}
\hat{\hat{A}}_{Qg}^{(3)} = {}& \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}\Bigg[\frac{\hat{\gamma}_{qg}^{(0)}}{6\varepsilon^3}\Big((n_f+1)\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + \gamma_{qq}^{(0)}\big[\gamma_{qq}^{(0)} - 2\gamma_{gg}^{(0)} - 6\beta_0 - 8\beta_{0,Q}\big] + 8\beta_0^2 \\
&+ 28\beta_{0,Q}\beta_0 + 24\beta_{0,Q}^2 + \gamma_{gg}^{(0)}\big[\gamma_{gg}^{(0)} + 6\beta_0 + 14\beta_{0,Q}\big]\Big) \\
&+ \frac{1}{6\varepsilon^2}\Big(\hat{\gamma}_{qg}^{(1)}\big[2\gamma_{qq}^{(0)} - 2\gamma_{gg}^{(0)} - 8\beta_0 - 10\beta_{0,Q}\big] \\
&+ \hat{\gamma}_{qg}^{(0)}\big[\hat{\gamma}_{qq}^{(1),\mathsf{PS}}\{1-2n_f\} + \gamma_{qq}^{(1),\mathsf{NS}} + \hat{\gamma}_{qq}^{(1),\mathsf{NS}} + 2\hat{\gamma}_{gg}^{(1)} - \gamma_{gg}^{(1)} - 2\beta_1 - 2\beta_{1,Q}\big] \\
&+ 6\delta m_1^{(-1)}\hat{\gamma}_{qg}^{(0)}\big[\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 3\beta_0 + 5\beta_{0,Q}\big]\Big) \\
&+ \frac{1}{\varepsilon}\Bigg(\frac{\hat{\gamma}_{qg}^{(2)}}{3} - n_f\frac{\hat{\tilde{\gamma}}_{qg}^{(2)}}{3} + \hat{\gamma}_{qg}^{(0)}\big[a_{gg,Q}^{(2)} - n_f a_{Qq}^{(2),\mathsf{PS}}\big] \\
&+ a_{Qg}^{(2)}\big[\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} - 4\beta_0 - 4\beta_{0,Q}\big] + \frac{\hat{\gamma}_{qg}^{(0)}\zeta_2}{16}\big[\gamma_{gg}^{(0)}\{2\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} - 6\beta_0 + 2\beta_{0,Q}\} \\
&- (n_f+1)\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + \gamma_{qq}^{(0)}\{-\gamma_{qq}^{(0)} + 6\beta_0\} - 8\beta_0^2 + 4\beta_{0,Q}\beta_0 + 24\beta_{0,Q}^2\big] \\
&+ \frac{\delta m_1^{(-1)}}{2}\big[-2\hat{\gamma}_{qg}^{(1)} + 3\delta m_1^{(-1)}\hat{\gamma}_{qg}^{(0)} + 2\delta m_1^{(0)}\hat{\gamma}_{qg}^{(0)}\big] \\
&+ \delta m_1^{(0)}\hat{\gamma}_{qg}^{(0)}\big[\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0 + 4\beta_{0,Q}\big] - \delta m_2^{(-1)}\hat{\gamma}_{qg}^{(0)}\Bigg) + a_{Qg}^{(3)}\Bigg], \qquad (4.37)
\end{aligned}
$$

$$
\begin{aligned}
\hat{\hat{A}}_{qg,Q}^{(3)} = {}& n_f\left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}\Bigg[\frac{\hat{\gamma}_{qg}^{(0)}}{6\varepsilon^3}\Big(\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + 2\beta_{0,Q}\big[\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0\big]\Big) \\
&+ \frac{1}{\varepsilon^2}\left(\frac{\hat{\gamma}_{qg}^{(0)}}{6}\big[2\hat{\gamma}_{gg}^{(1)} + \hat{\gamma}_{qq}^{(1),\mathsf{PS}} - 2\hat{\gamma}_{qq}^{(1),\mathsf{NS}} + 4\beta_{1,Q}\big] + \frac{\hat{\gamma}_{qg}^{(1)}\beta_{0,Q}}{3}\right) \\
&+ \frac{1}{\varepsilon}\Bigg(\frac{\hat{\tilde{\gamma}}_{qg}^{(2)}}{3} + \hat{\gamma}_{qg}^{(0)}\big[a_{gg,Q}^{(2)} - a_{qq,Q}^{(2),\mathsf{NS}} + \beta_{1,Q}^{(1)}\big] \\
&- \frac{\hat{\gamma}_{qg}^{(0)}\zeta_2}{16}\big[\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + 2\beta_{0,Q}\{\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0\}\big]\Bigg) + \frac{a_{qg,Q}^{(3)}}{n_f}\Bigg]. \qquad (4.38)
\end{aligned}
$$

The renormalized expressions are

$$
\begin{aligned}
A_{Qg}^{(3),\overline{\mathsf{MS}}} = {} & \frac{\hat{\gamma}_{qg}^{(0)}}{48}\big\{(n_f+1)\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + \gamma_{gg}^{(0)}\big(\gamma_{gg}^{(0)} - 2\gamma_{qq}^{(0)} + 6\beta_0 + 14\beta_{0,Q}\big) \\
& + \gamma_{qq}^{(0)}\big(\gamma_{qq}^{(0)} - 6\beta_0 - 8\beta_{0,Q}\big) + 8\beta_0^2 + 28\beta_{0,Q}\beta_0 + 24\beta_{0,Q}^2\big\}\ln^3\left(\frac{m^2}{\mu^2}\right) \\
& + \frac{1}{8}\big\{\hat{\gamma}_{qg}^{(1)}\big(\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} - 4\beta_0 - 6\beta_{0,Q}\big) + \hat{\gamma}_{qg}^{(0)}\big(\hat{\gamma}_{gg}^{(1)} - \gamma_{gg}^{(1)} + (1-n_f)\hat{\gamma}_{qq}^{(1),\mathsf{PS}} \\
& + \gamma_{qq}^{(1),\mathsf{NS}} + \hat{\gamma}_{qq}^{(1),\mathsf{NS}} - 2\beta_1 - 2\beta_{1,Q}\big)\big\}\ln^2\left(\frac{m^2}{\mu^2}\right) \\
& + \left\{\frac{\hat{\gamma}_{qg}^{(2)}}{2} - n_f\frac{\hat{\hat{\gamma}}_{qg}^{(2)}}{2} + \frac{a_{Qg}^{(2)}}{2}\big(\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} - 4\beta_0 - 4\beta_{0,Q}\big)\right. \\
& + \frac{\hat{\gamma}_{qg}^{(0)}}{2}\big(a_{gg,Q}^{(2)} - n_f a_{Qq}^{(2),\mathsf{PS}}\big) + \frac{\hat{\gamma}_{qg}^{(0)}\zeta_2}{16}\big(-(n_f+1)\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} \\
& + \gamma_{gg}^{(0)}\big[2\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} - 6\beta_0 - 6\beta_{0,Q}\big] - 4\beta_0[2\beta_0 + 3\beta_{0,Q}] \\
& \left. + \gamma_{qq}^{(0)}\big[-\gamma_{qq}^{(0)} + 6\beta_0 + 4\beta_{0,Q}\big]\big)\right\}\ln\left(\frac{m^2}{\mu^2}\right) + \bar{a}_{Qg}^{(2)}\big(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 4\beta_0 + 4\beta_{0,Q}\big) \\
& + \hat{\gamma}_{qg}^{(0)}\big(n_f\bar{a}_{Qq}^{(2),\mathsf{PS}} - \bar{a}_{gg,Q}^{(2)}\big) + \frac{\hat{\gamma}_{qg}^{(0)}\zeta_3}{48}\big((n_f+1)\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} \\
& + \gamma_{gg}^{(0)}\big[\gamma_{gg}^{(0)} - 2\gamma_{qq}^{(0)} + 6\beta_0 - 2\beta_{0,Q}\big] \\
& + \gamma_{qq}^{(0)}\big[\gamma_{qq}^{(0)} - 6\beta_0\big] + 8\beta_0^2 - 4\beta_0\beta_{0,Q} - 24\beta_{0,Q}^2\big) \\
& + \frac{\hat{\gamma}_{qg}^{(1)}\beta_{0,Q}\zeta_2}{8} + \frac{\hat{\gamma}_{qg}^{(0)}\zeta_2}{16}\big(\gamma_{gg}^{(1)} - \hat{\gamma}_{qq}^{(1),\mathsf{NS}} - \gamma_{qq}^{(1),\mathsf{NS}} - \hat{\gamma}_{qq}^{(1),\mathsf{PS}} + 2\beta_1 + 2\beta_{1,Q}\big) \\
& + \frac{\delta m_1^{(-1)}}{8}\big(16a_{Qg}^{(2)} + \hat{\gamma}_{qg}^{(0)}\big[-24\delta m_1^{(0)} - 8\delta m_1^{(1)} - \zeta_2\beta_0 - 9\zeta_2\beta_{0,Q}\big]\big) \\
& + \frac{\delta m_1^{(0)}}{2}\big(2\hat{\gamma}_{qg}^{(1)} - \delta m_1^{(0)}\hat{\gamma}_{qg}^{(0)}\big) + \delta m_1^{(1)}\hat{\gamma}_{qg}^{(0)}\big(\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} - 2\beta_0 - 4\beta_{0,Q}\big) \\
& + \delta m_2^{(0)}\hat{\gamma}_{qg}^{(0)} + a_{Qg}^{(3)},
\end{aligned}
\tag{4.39}
$$

$$
\begin{aligned}
A_{qg,Q}^{(3),\overline{\mathsf{MS}}} = {} & n_f\left[\frac{\hat{\gamma}_{qg}^{(0)}}{48}\big\{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + 2\beta_{0,Q}\big(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0\big)\big\}\ln^3\left(\frac{m^2}{\mu^2}\right)\right. \\
& + \frac{1}{8}\big\{2\hat{\gamma}_{qg}^{(1)}\beta_{0,Q} + \hat{\gamma}_{qg}^{(0)}\big(\hat{\gamma}_{qq}^{(1),\mathsf{PS}} - \hat{\gamma}_{qq}^{(1),\mathsf{NS}} + \hat{\gamma}_{gg}^{(1)} + 2\beta_{1,Q}\big)\big\}\ln^2\left(\frac{m^2}{\mu^2}\right) \\
& + \frac{1}{2}\left\{\hat{\hat{\gamma}}_{qg}^{(2)} + \hat{\gamma}_{qg}^{(0)}\big(a_{gg,Q}^{(2)} - a_{qq,Q}^{(2),\mathsf{NS}} + \beta_{1,Q}^{(1)}\big)\right. \\
& \left. - \frac{\hat{\gamma}_{qg}^{(0)}}{8}\zeta_2\big(\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + 2\beta_{0,Q}\big[\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 2\beta_0\big]\big)\right\}\ln\left(\frac{m^2}{\mu^2}\right) \\
& + \hat{\gamma}_{qg}^{(0)}\big(\bar{a}_{qq,Q}^{(2),\mathsf{NS}} - \bar{a}_{gg,Q}^{(2)} - \beta_{1,Q}^{(2)}\big)
\end{aligned}
$$

$$+\frac{\hat{\gamma}_{qg}^{(0)}}{48}\zeta_3\big(\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}+2\beta_{0,Q}\big[\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+2\beta_0\big]\big)$$
$$-\frac{\zeta_2}{16}\big(\hat{\gamma}_{qg}^{(0)}\hat{\gamma}_{qq}^{(1),\mathsf{PS}}+2\hat{\gamma}_{qg}^{(1)}\beta_{0,Q}\big)+\frac{a_{qg,Q}^{(3)}}{n_f}\Bigg]. \tag{4.40}$$

4.5. $A_{gq,Q}$

The gq-contributions start at $O(a_s^2)$,

$$A_{gq,Q}=a_s^2A_{gq,Q}^{(2)}+a_s^3A_{gq,Q}^{(3)}+O\big(a_s^4\big). \tag{4.41}$$

The renormalization formulae in the MOM-scheme read

$$\begin{aligned}A_{gq,Q}^{(2),\mathsf{MOM}}&=\hat{A}_{gq,Q}^{(2),\mathsf{MOM}}+Z_{gq}^{-1,(2)}(n_f+1)-Z_{gq}^{-1,(2)}(n_f)\\&\quad+\big(\hat{A}_{gg,Q}^{(1),\mathsf{MOM}}+Z_{gg}^{-1,(1)}(n_f+1)-Z_{gg}^{-1,(1)}(n_f)\big)\Gamma_{gq}^{-1,(1)},\end{aligned} \tag{4.42}$$

$$\begin{aligned}A_{gq,Q}^{(3),\mathsf{MOM}}&=\hat{A}_{gq,Q}^{(3),\mathsf{MOM}}+Z_{gq}^{-1,(3)}(n_f+1)-Z_{gq}^{-1,(3)}(n_f)+Z_{gg}^{-1,(1)}(n_f+1)\hat{A}_{gq,Q}^{(2),\mathsf{MOM}}\\&\quad+Z_{gq}^{-1,(1)}(n_f+1)\hat{A}_{qq}^{(2),\mathsf{MOM}}+\big[\hat{A}_{gg,Q}^{(1),\mathsf{MOM}}+Z_{gg}^{-1,(1)}(n_f+1)\\&\quad-Z_{gg}^{-1,(1)}(n_f)\big]\Gamma_{gq}^{-1,(2)}(n_f)\\&\quad+\big[\hat{A}_{gq,Q}^{(2),\mathsf{MOM}}+Z_{gq}^{-1,(2)}(n_f+1)-Z_{gq}^{-1,(2)}(n_f)\big]\Gamma_{qq}^{-1,(1)}(n_f)\\&\quad+\big[\hat{A}_{gg,Q}^{(2),\mathsf{MOM}}+Z_{gg}^{-1,(2)}(n_f+1)-Z_{gg}^{-1,(2)}(n_f)+Z_{gg}^{-1,(1)}(n_f+1)\hat{A}_{gg,Q}^{(1),\mathsf{MOM}}\\&\quad+Z_{gq}^{-1,(1)}(n_f+1)\hat{A}_{Qg}^{(1),\mathsf{MOM}}\big]\Gamma_{gq}^{-1,(1)}(n_f),\end{aligned} \tag{4.43}$$

while the unrenormalized expressions are

$$\hat{\hat{A}}_{gq,Q}^{(2)}=\left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\left[\frac{2\beta_{0,Q}}{\varepsilon^2}\gamma_{gq}^{(0)}+\frac{\hat{\gamma}_{gq}^{(1)}}{2\varepsilon}+a_{gq,Q}^{(2)}+\bar{a}_{gq,Q}^{(2)}\varepsilon\right], \tag{4.44}$$

$$\begin{aligned}\hat{\hat{A}}_{gq,Q}^{(3)}&=\left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}\Bigg\{-\frac{\gamma_{gq}^{(0)}}{3\varepsilon^3}\big(\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}+\big[\gamma_{qq}^{(0)}-\gamma_{gg}^{(0)}+10\beta_0+24\beta_{0,Q}\big]\beta_{0,Q}\big)\\&\quad+\frac{1}{\varepsilon^2}\Bigg(\gamma_{gq}^{(1)}\beta_{0,Q}+\frac{\hat{\gamma}_{gq}^{(1)}}{3}\big[\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}-4\beta_0-6\beta_{0,Q}\big]\\&\quad+\frac{\gamma_{gq}^{(0)}}{3}\big[\hat{\gamma}_{qq}^{(1),\mathsf{NS}}+\hat{\gamma}_{qq}^{(1),\mathsf{PS}}-\hat{\gamma}_{gg}^{(1)}+2\beta_{1,Q}\big]-4\delta m_1^{(-1)}\beta_{0,Q}\gamma_{gq}^{(0)}\Bigg)\\&\quad+\frac{1}{\varepsilon}\Bigg(\frac{\hat{\gamma}_{gq}^{(2)}}{3}+a_{gq,Q}^{(2)}\big[\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}-6\beta_{0,Q}-4\beta_0\big]\\&\quad+\gamma_{gq}^{(0)}\big[a_{qq,Q}^{(2),\mathsf{NS}}+a_{Qq}^{(2),\mathsf{PS}}-a_{gg,Q}^{(2)}\big]+\gamma_{gq}^{(0)}\beta_{1,Q}^{(1)}\\&\quad+\frac{\gamma_{gq}^{(0)}\zeta_2}{8}\big[\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}+\beta_{0,Q}\big(\gamma_{qq}^{(0)}-\gamma_{gg}^{(0)}+10\beta_0\big)\big]-\delta m_1^{(-1)}\hat{\gamma}_{gq}^{(1)}\\&\quad-4\delta m_1^{(0)}\beta_{0,Q}\gamma_{gq}^{(0)}\Bigg)+a_{gq,Q}^{(3)}\Bigg\}.\end{aligned} \tag{4.45}$$

The contributions to the renormalized operator matrix element are given by

$$A_{gq,Q}^{(2),\overline{\mathsf{MS}}} = \frac{\beta_{0,Q}\gamma_{gq}^{(0)}}{2}\ln^2\left(\frac{m^2}{\mu^2}\right) + \frac{\hat{\gamma}_{gq}^{(1)}}{2}\ln\left(\frac{m^2}{\mu^2}\right) + a_{gq,Q}^{(2)} - \frac{\beta_{0,Q}\gamma_{gq}^{(0)}}{2}\zeta_2, \tag{4.46}$$

$$\begin{aligned}
A_{gq,Q}^{(3),\overline{\mathsf{MS}}} = & -\frac{\gamma_{gq}^{(0)}}{24}\left\{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + \left(\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} + 10\beta_0 + 24\beta_{0,Q}\right)\beta_{0,Q}\right\}\ln^3\left(\frac{m^2}{\mu^2}\right) \\
& + \frac{1}{8}\left\{6\gamma_{gq}^{(1)}\beta_{0,Q} + \hat{\gamma}_{gq}^{(1)}\left(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} - 4\beta_0 - 6\beta_{0,Q}\right)\right. \\
& \left. + \gamma_{gq}^{(0)}\left(\hat{\gamma}_{qq}^{(1),\mathsf{NS}} + \hat{\gamma}_{qq}^{(1),\mathsf{PS}} - \hat{\gamma}_{gg}^{(1)} + 2\beta_{1,Q}\right)\right\}\ln^2\left(\frac{m^2}{\mu^2}\right) \\
& + \frac{1}{8}\left\{4\hat{\gamma}_{gq}^{(2)} + 4a_{gq,Q}^{(2)}\left(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} - 4\beta_0 - 6\beta_{0,Q}\right)\right. \\
& + 4\gamma_{gq}^{(0)}\left(a_{qq,Q}^{(2),\mathsf{NS}} + a_{Qq}^{(2),\mathsf{PS}} - a_{gg,Q}^{(2)} + \beta_{1,Q}^{(1)}\right) + \gamma_{gq}^{(0)}\zeta_2\left(\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\right. \\
& \left.\left. + \left[\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} + 12\beta_{0,Q} + 10\beta_0\right]\beta_{0,Q}\right)\right\}\ln\left(\frac{m^2}{\mu^2}\right) \\
& + \bar{a}_{gq,Q}^{(2)}\left(\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} + 4\beta_0 + 6\beta_{0,Q}\right) \\
& + \gamma_{gq}^{(0)}\left(\bar{a}_{gg,Q}^{(2)} - \bar{a}_{Qq}^{(2),\mathsf{PS}} - \bar{a}_{qq,Q}^{(2),\mathsf{NS}}\right) - \gamma_{gq}^{(0)}\beta_{1,Q}^{(2)} \\
& - \frac{\gamma_{gq}^{(0)}\zeta_3}{24}\left(\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + \left[\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} + 10\beta_0\right]\beta_{0,Q}\right) - \frac{3\gamma_{gq}^{(1)}\beta_{0,Q}\zeta_2}{8} \\
& + 2\delta m_1^{(-1)} a_{gq,Q}^{(2)} + \delta m_1^{(0)}\hat{\gamma}_{gq}^{(1)} + 4\delta m_1^{(1)}\beta_{0,Q}\gamma_{gq}^{(0)} + a_{gq,Q}^{(3)}.
\end{aligned} \tag{4.47}$$

4.6. $A_{gg,Q}$

The gg-contributions start at $O(a_s)$,

$$A_{gg,Q} = a_s A_{gg,Q}^{(1)} + a_s^2 A_{gg,Q}^{(2)} + a_s^3 A_{gg,Q}^{(3)} + O\left(a_s^4\right). \tag{4.48}$$

The corresponding renormalization formulae read in the MOM-scheme

$$A_{gg,Q}^{(1),\mathsf{MOM}} = \hat{A}_{gg,Q}^{(1),\mathsf{MOM}} + Z_{gg}^{-1,(1)}(n_f+1) - Z_{gg}^{-1,(1)}(n_f), \tag{4.49}$$

$$\begin{aligned}
A_{gg,Q}^{(2),\mathsf{MOM}} = & \hat{A}_{gg,Q}^{(2),\mathsf{MOM}} + Z_{gg}^{-1,(2)}(n_f+1) - Z_{gg}^{-1,(2)}(n_f) + Z_{gg}^{-1,(1)}(n_f+1)\hat{A}_{gg,Q}^{(1),\mathsf{MOM}} \\
& + Z_{gq}^{-1,(1)}(n_f+1)\hat{A}_{Qg}^{(1),\mathsf{MOM}} \\
& + \left[\hat{A}_{gg,Q}^{(1),\mathsf{MOM}} + Z_{gg}^{-1,(1)}(n_f+1) - Z_{gg}^{-1,(1)}(n_f)\right]\Gamma_{gg}^{-1,(1)}(n_f),
\end{aligned} \tag{4.50}$$

$$\begin{aligned}
A_{gg,Q}^{(3),\mathsf{MOM}} = & \hat{A}_{gg,Q}^{(3),\mathsf{MOM}} + Z_{gg}^{-1,(3)}(n_f+1) - Z_{gg}^{-1,(3)}(n_f) + Z_{gg}^{-1,(2)}(n_f+1)\hat{A}_{gg,Q}^{(1),\mathsf{MOM}} \\
& + Z_{gg}^{-1,(1)}(n_f+1)\hat{A}_{gg,Q}^{(2),\mathsf{MOM}} + Z_{gq}^{-1,(2)}(n_f+1)\hat{A}_{Qg}^{(1),\mathsf{MOM}} \\
& + Z_{gq}^{-1,(1)}(n_f+1)\hat{A}_{Qg}^{(2),\mathsf{MOM}} \\
& + \left[\hat{A}_{gg,Q}^{(1),\mathsf{MOM}} + Z_{gg}^{-1,(1)}(n_f+1) - Z_{gg}^{-1,(1)}(n_f)\right]\Gamma_{gg}^{-1,(2)}(n_f) \\
& + \left[\hat{A}_{gg,Q}^{(2),\mathsf{MOM}} + Z_{gg}^{-1,(2)}(n_f+1) - Z_{gg}^{-1,(2)}(n_f) + Z_{gq}^{-1,(1)}(n_f+1)A_{Qg}^{(1),\mathsf{MOM}}\right. \\
& \left. + Z_{gg}^{-1,(1)}(n_f+1)A_{gg,Q}^{(1),\mathsf{MOM}}\right]\Gamma_{gg}^{-1,(1)}(n_f)
\end{aligned}$$

$$+\big[\hat{A}_{gq,Q}^{(2),\mathrm{MOM}}+Z_{gq}^{-1,(2)}(n_f+1)-Z_{gq}^{-1,(2)}(n_f)\big]\Gamma_{qg}^{-1,(1)}(n_f). \tag{4.51}$$

The general structure of the unrenormalized 1-loop result is then given by

$$\hat{\hat{A}}_{gg,Q}^{(1)}=\left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2}\left(\frac{\hat{\gamma}_{gg}^{(0)}}{\varepsilon}+a_{gg,Q}^{(1)}+\varepsilon\bar{a}_{gg,Q}^{(1)}+\varepsilon^2\bar{\bar{a}}_{gg,Q}^{(1)}\right). \tag{4.52}$$

An explicit calculation reveals

$$\hat{\hat{A}}_{gg,Q}^{(1)}=\left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2}\left(-\frac{2\beta_{0,Q}}{\varepsilon}\right)\exp\left(\sum_{i=2}^{\infty}\frac{\zeta_i}{i}\left(\frac{\varepsilon}{2}\right)^i\right). \tag{4.53}$$

Using Eq. (4.53), the 2-loop term is given by

$$\hat{\hat{A}}_{gg,Q}^{(2)}=\left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\left[\frac{1}{2\varepsilon^2}\left\{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}+2\beta_{0,Q}\left(\gamma_{gg}^{(0)}+2\beta_0+4\beta_{0,Q}\right)\right\}+\frac{\hat{\gamma}_{gg}^{(1)}+4\delta m_1^{(-1)}\beta_{0,Q}}{2\varepsilon}\right.$$
$$\left.+a_{gg,Q}^{(2)}+2\delta m_1^{(0)}\beta_{0,Q}+\beta_{0,Q}^2\zeta_2+\varepsilon\left[\bar{a}_{gg,Q}^{(2)}+2\delta m_1^{(1)}\beta_{0,Q}+\frac{\beta_{0,Q}^2\zeta_3}{6}\right]\right]. \tag{4.54}$$

For Eq. (4.54) the same as for Eq. (4.33) holds. We have already included one-particle reducible contributions and terms stemming from mass renormalization in order to refer to the notation of Refs. [29,31]. The 3-loop contribution becomes

$$\hat{\hat{A}}_{gg,Q}^{(3)}=\left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}\left[\frac{1}{\varepsilon^3}\left(-\frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}}{6}\left[\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0+4n_f\beta_{0,Q}+10\beta_{0,Q}\right]\right.\right.$$
$$\left.-\frac{2\gamma_{gg}^{(0)}\beta_{0,Q}}{3}\left[2\beta_0+7\beta_{0,Q}\right]-\frac{4\beta_{0,Q}}{3}\left[2\beta_0^2+7\beta_{0,Q}\beta_0+6\beta_{0,Q}^2\right]\right)$$
$$+\frac{1}{\varepsilon^2}\left(\frac{\hat{\gamma}_{qg}^{(0)}}{6}\left[\gamma_{gq}^{(1)}-(2n_f-1)\hat{\gamma}_{gq}^{(1)}\right]+\frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(1)}}{3}-\frac{\hat{\gamma}_{gg}^{(1)}}{3}\left[4\beta_0+7\beta_{0,Q}\right]\right.$$
$$+\frac{2\beta_{0,Q}}{3}\left[\gamma_{gg}^{(1)}+\beta_1+\beta_{1,Q}\right]+\frac{2\gamma_{gg}^{(0)}\beta_{1,Q}}{3}$$
$$\left.+\delta m_1^{(-1)}\left[-\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}-2\beta_{0,Q}\gamma_{gg}^{(0)}-10\beta_{0,Q}^2-6\beta_{0,Q}\beta_0\right]\right)$$
$$+\frac{1}{\varepsilon}\left(\frac{\hat{\gamma}_{gg}^{(2)}}{3}-2(2\beta_0+3\beta_{0,Q})a_{gg,Q}^{(2)}-n_f\hat{\gamma}_{qg}^{(0)}a_{gq,Q}^{(2)}+\gamma_{gq}^{(0)}a_{Qg}^{(2)}+\beta_{1,Q}^{(1)}\gamma_{gg}^{(0)}\right.$$
$$+\frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\zeta_2}{16}\left[\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+2(2n_f+1)\beta_{0,Q}+6\beta_0\right]$$
$$+\frac{\beta_{0,Q}\zeta_2}{4}\left[\gamma_{gg}^{(0)}\{2\beta_0-\beta_{0,Q}\}+4\beta_0^2-2\beta_{0,Q}\beta_0-12\beta_{0,Q}^2\right]$$
$$+\delta m_1^{(-1)}\left[-3\delta m_1^{(-1)}\beta_{0,Q}-2\delta m_1^{(0)}\beta_{0,Q}-\hat{\gamma}_{gg}^{(1)}\right]$$
$$+\delta m_1^{(0)}\left[-\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}-2\gamma_{gg}^{(0)}\beta_{0,Q}-4\beta_{0,Q}\beta_0-8\beta_{0,Q}^2\right]$$
$$\left.\left.+2\delta m_2^{(-1)}\beta_{0,Q}\right)+a_{gg,Q}^{(3)}\right]. \tag{4.55}$$

The renormalized results are

$$A_{gg,Q}^{(1),\overline{\mathsf{MS}}} = -\beta_{0,Q} \ln\left(\frac{m^2}{\mu^2}\right), \tag{4.56}$$

$$\begin{aligned} A_{gg,Q}^{(2),\overline{\mathsf{MS}}} &= \frac{1}{8}\left\{2\beta_{0,Q}\left(\gamma_{gg}^{(0)}+2\beta_0\right)+\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}+8\beta_{0,Q}^2\right\}\ln^2\left(\frac{m^2}{\mu^2}\right)+\frac{\hat{\gamma}_{gg}^{(1)}}{2}\ln\left(\frac{m^2}{\mu^2}\right) \\ &\quad -\frac{\zeta_2}{8}\left[2\beta_{0,Q}\left(\gamma_{gg}^{(0)}+2\beta_0\right)+\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\right]+a_{gg,Q}^{(2)}, \end{aligned} \tag{4.57}$$

$$\begin{aligned} A_{gg,Q}^{(3),\overline{\mathsf{MS}}} &= \frac{1}{48}\left\{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\left(\gamma_{qq}^{(0)}-\gamma_{gg}^{(0)}-6\beta_0-4n_f\beta_{0,Q}-10\beta_{0,Q}\right)-4\left(\gamma_{gg}^{(0)}[2\beta_0+7\beta_{0,Q}]\right.\right. \\ &\quad \left.\left.+4\beta_0^2+14\beta_{0,Q}\beta_0+12\beta_{0,Q}^2\right)\beta_{0,Q}\right\}\ln^3\left(\frac{m^2}{\mu^2}\right)+\frac{1}{8}\left\{\hat{\gamma}_{qg}^{(0)}\left(\gamma_{gq}^{(1)}+(1-n_f)\hat{\gamma}_{gq}^{(1)}\right)\right. \\ &\quad +\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(1)}+4\gamma_{gg}^{(1)}\beta_{0,Q}-4\hat{\gamma}_{gg}^{(1)}[\beta_0+2\beta_{0,Q}]+2\gamma_{gg}^{(0)}\beta_{1,Q} \\ &\quad \left.+4[\beta_1+\beta_{1,Q}]\beta_{0,Q}\right\}\ln^2\left(\frac{m^2}{\mu^2}\right) \\ &\quad +\frac{1}{16}\left\{8\hat{\gamma}_{gg}^{(2)}-8n_f a_{gq,Q}^{(2)}\hat{\gamma}_{qg}^{(0)}-16a_{gg,Q}^{(2)}(2\beta_0+3\beta_{0,Q})\right. \\ &\quad +8\gamma_{gq}^{(0)}a_{Qg}^{(2)}+8\gamma_{gg}^{(0)}\beta_{1,Q}^{(1)} \\ &\quad +\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\zeta_2\left(\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0+4n_f\beta_{0,Q}+6\beta_{0,Q}\right) \\ &\quad \left.+4\beta_{0,Q}\zeta_2\left(\gamma_{gg}^{(0)}+2\beta_0\right)(2\beta_0+3\beta_{0,Q})\right\}\ln\left(\frac{m^2}{\mu^2}\right)+2(2\beta_0+3\beta_{0,Q})\bar{a}_{gg,Q}^{(2)} \\ &\quad +n_f\hat{\gamma}_{qg}^{(0)}\bar{a}_{gq,Q}^{(2)}-\gamma_{gq}^{(0)}\bar{a}_{Qg}^{(2)}-\beta_{1,Q}^{(2)}\gamma_{gg}^{(0)} \\ &\quad +\frac{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\zeta_3}{48}\left(\gamma_{qq}^{(0)}-\gamma_{gg}^{(0)}-2[2n_f+1]\beta_{0,Q}-6\beta_0\right) \\ &\quad +\frac{\beta_{0,Q}\zeta_3}{12}\left([\beta_{0,Q}-2\beta_0]\gamma_{gg}^{(0)}+2[\beta_0+6\beta_{0,Q}]\beta_{0,Q}-4\beta_0^2\right) \\ &\quad -\frac{\hat{\gamma}_{qg}^{(0)}\zeta_2}{16}\left(\gamma_{gq}^{(1)}+\hat{\gamma}_{gq}^{(1)}\right)+\frac{\beta_{0,Q}\zeta_2}{8}\left(\hat{\gamma}_{gg}^{(1)}-2\gamma_{gg}^{(1)}-2\beta_1-2\beta_{1,Q}\right) \\ &\quad +\frac{\delta m_1^{(-1)}}{4}\left(8a_{gg,Q}^{(2)}+24\delta m_1^{(0)}\beta_{0,Q}+8\delta m_1^{(1)}\beta_{0,Q}+\zeta_2\beta_{0,Q}\beta_0+9\zeta_2\beta_{0,Q}^2\right) \\ &\quad +\delta m_1^{(0)}\left(\beta_{0,Q}\delta m_1^{(0)}+\hat{\gamma}_{gg}^{(1)}\right) \\ &\quad +\delta m_1^{(1)}\left(\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}+2\beta_{0,Q}\gamma_{gg}^{(0)}+4\beta_{0,Q}\beta_0+8\beta_{0,Q}^2\right) \\ &\quad -2\delta m_2^{(0)}\beta_{0,Q}+a_{gg,Q}^{(3)}. \end{aligned} \tag{4.58}$$

5. The calculation of the operator matrix elements

In this chapter, we describe the computation of the 3-loop corrections to the massive operator matrix elements in detail. Typical Feynman diagrams contributing to the different channels are shown in Fig. 1, where ⊗ denotes the corresponding composite operator insertions, (2.7)–(2.9).

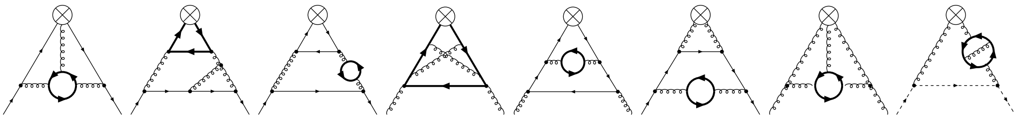

Fig. 1. Examples for 3-loop diagrams contributing to the massive operator matrix elements: NS — non-singlet, $\mathsf{PS}_{\mathsf{H},l}$ — pure-singlet, singlet $qg_{H,l}$, gq, gg and ghost contributions. Here the coupling of the gauge boson to a heavy or light fermion line is labeled by H and l, respectively. Thick lines: heavy quarks, curly lines: gluons, full lines: quarks, dashed lines: ghosts.

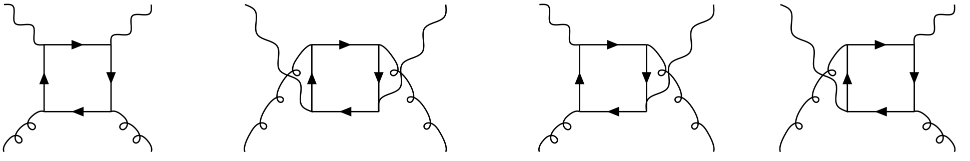

Fig. 2. Diagrams contributing to $A_{Qg}^{(1)}$ via the optical theorem. Wavy lines denote photons; for the other lines, see Fig. 1.

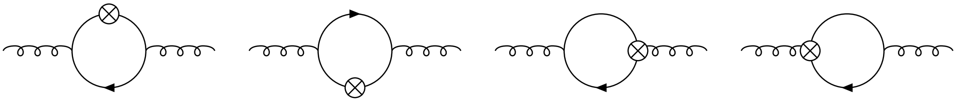

Fig. 3. Diagrams contributing to $A_{Qg}^{(1)}$.

The generation of these diagrams with the FORTRAN-based program QGRAF, cf. [63], is described in Section 5.1 along with the subsequent steps to prepare the input for the FORM-based program MATAD [60]. The latter allows the calculation of massive tadpole integrals in D dimensions up to three loops and relies on the MINCER algorithm [64,65]. The use of MATAD and the projection onto fixed moments are explained in Section 5.2. Finally, we present our results for the fixed moments of the 3-loop OMEs and the fermionic contributions to the anomalous dimensions in Section 5.3. The calculation is mainly performed by using FORM programs [66], while in a few cases codes have also been written in MAPLE.

5.1. Generation of diagrams

QGRAF is a quite general program to generate Feynman diagrams and allows to specify various kinds of particles and interactions. Our main issue is to generate diagrams which contain composite operator insertions, cf. (2.7)–(2.9) and Appendix A.1, as special vertices.

To give an example, let us consider the contributions to $A_{Qg}^{(1)}$. Within the light-cone expansion [67], this term derives from the Born diagrams squared of the photon–gluon fusion process shown in Fig. 2. After expanding these diagrams with respect to the virtuality of the photon, the mass effects are then given by the diagrams in Fig. 3. These are obtained by contracting the lines between the external photons. Thus, one may think of the operator insertion as being coupled to two external particles, an incoming and an outgoing one, which carry the same momentum. Therefore, one defines in the model file of QGRAF vertices which resemble the operator insertions in this manner, using a scalar field ϕ, which shall not propagate in order to ensure that

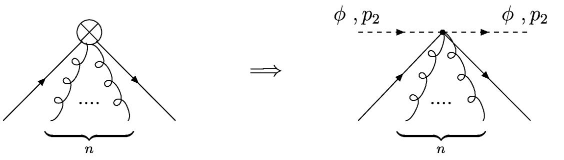

Fig. 4. Generation of the operator insertion.

Table 1
Number of diagrams contributing to the 3-loop heavy OMEs.

Term	#	Term	#	Term	#	Term	#
$A_{Qg}^{(3)}$	1358	$A_{qg,Q}^{(3)}$	140	$A_{Qq}^{(3),\mathsf{PS}}$	125	$A_{qq,Q}^{(3),\mathsf{PS}}$	8
$A_{qq,Q}^{(3),\mathsf{NS}}$	129	$A_{gq,Q}^{(3)}$	89	$A_{gg,Q}^{(3)}$	886		

Fig. 5. 2-Loop topologies, indicating labeling of momenta.

there is only one of these vertices for each diagram. For the quarkonic operators, one defines the vertices

$$\phi + \phi + q + \bar{q} + ng, \quad 0 \leqslant n \leqslant 3, \tag{5.1}$$

which is illustrated in Fig. 4. The same procedure can be used for the purely gluonic interactions and one defines in this case

$$\phi + \phi + ng, \quad 0 \leqslant n \leqslant 4. \tag{5.2}$$

The number of diagrams we obtain contributing to each OME is shown in Table 1. The next step consists in rewriting the output provided by QGRAF in such a way, that the Feynman rules given in Appendix A.1 can be inserted. Thus, one has to introduce Lorentz and color indices and align the fermion lines. Additionally, the integration momenta have to be written in such a way that MATAD can handle them. For the latter step, all information on the types of particles, the operator insertion and the external momentum are irrelevant, leading to only two basic topologies to be considered at the 2-loop level, which are shown in Fig. 5. Note, that in the case at hand the topology on the right-hand side of Fig. 5 always yields zero after integration. At the 3-loop level, the master topology is given in Fig. 6. From this topology, five types of diagrams are derived by shrinking various lines. These diagrams are shown in Fig. 7. After assigning the loop momenta, the Feynman rules are inserted. The computation of the Green's functions, which are associated to the respective operator matrix elements, still contain trace terms and require the symmetrization of the Lorentz indices. It is convenient to project these terms out by multiplying with an external source

$$J_N \equiv \Delta_{\mu_1} \cdots \Delta_{\mu_N}, \tag{5.3}$$

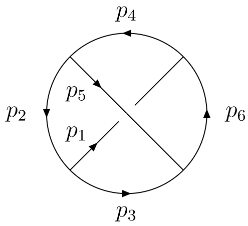

Fig. 6. Master 3-loop topology for MATAD, indicating labeling of momenta.

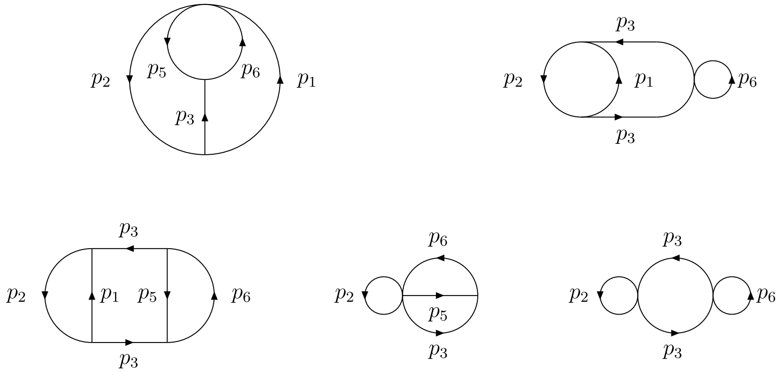

Fig. 7. Additional topologies contributing at the 3-loop level.

with Δ_μ being a light-like vector, $\Delta^2 = 0$. Additionally, one has to amputate the external field.[9] The Green's functions in momentum space corresponding to the local operators defined in Eqs. (2.8), (2.9) between gluonic states are then given by

$$\epsilon^\mu(p) G^{ab}_{Q,\mu\nu} \epsilon^\nu(p) = J_N \epsilon^\mu(p) \langle A^a_\mu(p) | O_Q^{\mu_1 \cdots \mu_N}(0) | A^b_\nu(p) \rangle \epsilon^\nu(p), \tag{5.4}$$

$$\epsilon^\mu(p) G^{ab}_{q,Q,\mu\nu} \epsilon^\nu(p) = J_N \epsilon^\mu(p) \langle A^a_\mu(p) | O_q^{\mu_1 \cdots \mu_N}(0) | A^b_\nu(p) \rangle_Q \epsilon^\nu(p), \tag{5.5}$$

$$\epsilon^\mu(p) G^{ab}_{g,Q,\mu\nu} \epsilon^\nu(p) = J_N \epsilon^\mu(p) \langle A^a_\mu(p) | O_g^{\mu_1 \cdots \mu_N}(0) | A^b_\nu(p) \rangle \epsilon^\nu(p), \tag{5.6}$$

cf. [29], with A^a_μ an external gluon field with color index a, Lorentz index μ, momentum p, and $\epsilon^\mu(p)$ the gluon polarization vector. In the flavor non-singlet case, Eq. (2.7), only one term contributes

$$\bar{u}(p,s) G_q^{ij,\mathsf{NS}} \lambda_r u(p,s) = J_N \langle \bar{\Psi}_i(p) | O_{q,r}^{\mu_1 \cdots \mu_N}(0) | \Psi^j(p) \rangle_Q, \tag{5.7}$$

with $u(p,s), \bar{u}(p,s)$ being the bi-spinors of the external quark and anti-quark, respectively. The remaining singlet and pure-singlet Green's functions with an external quark are given by [29],

$$\bar{u}(p,s) G_Q^{ij,\mathsf{S}} u(p,s) = J_N \langle \bar{\Psi}_i(p) | O_Q^{\mu_1 \cdots \mu_N}(0) | \Psi^j(p) \rangle, \tag{5.8}$$

$$\bar{u}(p,s) G_{q,Q}^{ij,\mathsf{S}} u(p,s) = J_N \langle \bar{\Psi}_i(p) | O_q^{\mu_1 \cdots \mu_N}(0) | \Psi^j(p) \rangle_Q, \tag{5.9}$$

[9] Note that we choose to renormalize the mass and the coupling multiplicatively and thus have to include self-energy insertions containing a massive line on external legs.

$$\bar{u}(p,s)G^{ij,\mathsf{S}}_{g,Q}u(p,s) = J_N\langle\bar{\Psi}_i(p)\big|O_g^{\mu_1\cdots\mu_N}(0)\big|\Psi^j(p)\rangle_Q. \tag{5.10}$$

Note, that in the quarkonic case the fields $\bar{\Psi}$, Ψ with color indices i, j stand for the external light quarks only. The above tensors have the general form, cf. [29,56],

$$G^{ab}_{l,\mu\nu} = \hat{\hat{A}}_{lg}\left(\frac{\hat{m}^2}{\mu^2},\varepsilon,N\right)\delta^{ab}(\Delta\cdot p)^N\left[-g_{\mu\nu} + \frac{p_\mu\Delta_\nu + \Delta_\mu p_\nu}{\Delta\cdot p}\right], \quad l = Q,g,q, \tag{5.11}$$

$$\hat{G}^{r,ij}_l = \hat{\hat{A}}^r_{lq}\left(\frac{\hat{m}^2}{\mu^2},\varepsilon,N\right)\delta^{ij}(\Delta\cdot p)^{N-1}\not{\Delta}, \quad l = Q,g,q,\ r = \mathsf{S},\mathsf{NS},\mathsf{PS}. \tag{5.12}$$

Here, $\hat{\hat{A}}_{ij}$ are the massive OMEs which we will calculate. In order to simplify this calculation, it is useful to define projection operators, which, applied to the Green's function, yield the corresponding OME. In the gluonic case, one defines

$$P^{(1),\mu\nu}_{ab;g}G^{ab}_{l,\mu\nu} \equiv -\frac{\delta_{ab}}{N_c^2-1}\frac{g^{\mu\nu}}{D-2}(\Delta\cdot p)^{-N}G^{ab}_{l,\mu\nu}, \tag{5.13}$$

$$P^{(2),\mu\nu}_{ab;g}G^{ab}_{l,\mu\nu} \equiv \frac{\delta_{ab}}{N_c^2-1}\frac{1}{D-2}(\Delta\cdot p)^{-N}\left(-g^{\mu\nu} + \frac{p^\mu\Delta^\nu + p^\nu\Delta^\mu}{\Delta\cdot p}\right)G^{ab}_{l,\mu\nu}. \tag{5.14}$$

In the quarkonic case, there is only one projector

$$P_{ij;q}G^{ij}_l \equiv \frac{\delta_{ij}}{N_c}(\Delta\cdot p)^{-N}\frac{1}{4}\mathrm{Tr}\big[\not{p}G^{ij}_l\big]. \tag{5.15}$$

The unrenormalized OMEs are given by

$$\hat{\hat{A}}_{lg}\left(\frac{\hat{m}^2}{\mu^2},\varepsilon,N\right) = P^{(1,2),\mu\nu}_{ab;g}G^{ab}_{l,\mu\nu}, \tag{5.16}$$

$$\hat{\hat{A}}_{lq}\left(\frac{\hat{m}^2}{\mu^2},\varepsilon,N\right) = P_{ij;q}G^{ij}_l. \tag{5.17}$$

These projections yield the advantage that one does not have to resort to complicated tensorial reductions. In perturbation theory, the expressions (5.16), (5.17) can then be evaluated order by order in the coupling constant by applying the Feynman rules given in Appendix A.1. While the projector (5.13) includes unphysical transverse gluon states, which have to be compensated adding the corresponding ghost-diagrams, (5.14) projects onto the physical states.

To calculate the color factor of each diagram, we use the program provided in Ref. [68]. Up to this point, all operations have been performed for general values of Mellin N and the dimensional parameter ε. The integrals do not contain any Lorentz or color indices anymore. In order to use MATAD, one now has to assign to N a specific value. Additionally, the unphysical momentum Δ has to be eliminated by applying a suitable projector, which we define in the following section.

5.2. *Calculation of fixed 3-loop moments using MATAD*

We consider integrals of the type

$$I_l(p,m,n_1,\ldots,n_j) \equiv \int\frac{d^Dk_1}{(2\pi)^D}\cdots\int\frac{d^Dk_l}{(2\pi)^D}(\Delta\,.\,q_1)^{n_1}\cdots(\Delta\,.\,q_j)^{n_j}f(k_1,\ldots,k_l,p,m). \tag{5.18}$$

Here p denotes the external momentum, $p^2 = 0$, m is the heavy quark mass, and Δ is a light-like vector, $\Delta^2 = 0$. The momenta q_i are given by any linear combination of the loop momenta k_i and external momentum p. The exponents n_i are integers or possibly sums of integers, see the Feynman rules in Appendix A.1. Their sum is given by

$$\sum_{i=1}^{j} n_i = N. \tag{5.19}$$

The function f in Eq. (5.18) contains propagators, of which at least one is massive, dot-products of its arguments and powers of m. If one sets $N = 0$, (5.18) becomes

$$I_l(p, m, 0, \ldots, 0) = I_l(m) = \int \frac{d^D k_1}{(2\pi)^D} \cdots \int \frac{d^D k_l}{(2\pi)^D} f(k_1, \ldots, k_l, m). \tag{5.20}$$

From $p^2 = 0$ it follows, that the result cannot depend on p anymore. The above integral is a massive tadpole integral and thus of the type MATAD can process. Additionally, MATAD can calculate the integral up to a given order as a power series in p^2/m^2. Let us return to the general integral given in Eq. (5.18). One notes, that for fixed moments of N, each integral of this type splits up into one or more integrals of the same type with n_i being just integers. At this point, it is useful to recall that the auxiliary vector Δ has only been introduced to get rid of the trace terms of the expectation values of the composite operators and has no physical significance. By undoing the contraction with Δ, these terms appear again. Consider as an example

$$I_l(p, m, 2, 1) = \int \frac{d^D k_1}{(2\pi)^D} \cdots \int \frac{d^D k_l}{(2\pi)^D} (\Delta . q_1)^2 (\Delta . q_2) f(k_1, \ldots, k_l, p, m) \tag{5.21}$$

$$= \Delta^{\mu_1}\Delta^{\mu_2}\Delta^{\mu_3} \int \frac{d^D k_1}{(2\pi)^D} \cdots \int \frac{d^D k_l}{(2\pi)^D} q_{1,\mu_1} q_{1,\mu_2} q_{2,\mu_3} f(k_1, \ldots, k_l, p, m). \tag{5.22}$$

One notices that the way of distributing the indices in Eq. (5.22) is somewhat arbitrary, since due to the contraction with the totally symmetric tensor $\Delta^{\mu_1}\Delta^{\mu_2}\Delta^{\mu_3}$, the result of the corresponding tensor integral can be taken to be fully symmetric as well. This is achieved by distributing the indices among the q_i in all possible ways and dividing by the number of permutations one has used. Thus Eq. (5.22) becomes

$$I_l(p, m, 2, 1) = \Delta^{\mu_1}\Delta^{\mu_2}\Delta^{\mu_3} \frac{1}{3} \int \frac{d^D k_1}{(2\pi)^D} \cdots \int \frac{d^D k_l}{(2\pi)^D} (q_{1,\mu_2} q_{1,\mu_3} q_{2,\mu_1} + q_{1,\mu_1} q_{1,\mu_3} q_{2,\mu_2} + q_{1,\mu_1} q_{1,\mu_2} q_{2,\mu_3}) f(k_1, \ldots, k_l, p, m). \tag{5.23}$$

Generally speaking, the symmetrization of the tensor resulting from

$$\prod_{i=1}^{j} (\Delta . q_1)^{n_i} \tag{5.24}$$

can be achieved by shuffling indices [69–74], and dividing by the number of terms. The shuffle product is given by

$$C\Big[\underbrace{(k_1, \ldots, k_1)}_{n_1} \sqcup\!\sqcup \underbrace{(k_2, \ldots, k_2)}_{n_2} \sqcup\!\sqcup \cdots \sqcup\!\sqcup \underbrace{(k_I, \ldots, k_I)}_{n_I}\Big], \tag{5.25}$$

where C is the normalization constant

$$C = \binom{N}{n_1, \ldots, n_I}^{-1}. \tag{5.26}$$

As an example, the symmetrization of

$$q_{1,\mu_1} q_{1,\mu_2} q_{2,\mu_3} \tag{5.27}$$

can be inferred from Eq. (5.23). After undoing the contraction with Δ in integral (5.18) and shuffling the indices, one may make the following Ansatz for the result, which follows from the necessity of complete symmetry in the Lorentz indices

$$R_{\{\mu_1 \cdots \mu_N\}} \equiv \sum_{j=1}^{[N/2]+1} A_j \left(\prod_{k=1}^{j-1} g_{\{\mu_{2k}\mu_{2k-1}} \right) \left(\prod_{l=2j-1}^{N} p_{\mu_l\}} \right). \tag{5.28}$$

In the above equation, [ ] denotes the Gauss-bracket and { } symmetrization with respect to the indices enclosed and dividing by the number of terms, as outlined above. The first few terms are then given by

$$R_0 \equiv 1, \tag{5.29}$$

$$R_{\{\mu_1\}} = A_1 p_{\mu_1}, \tag{5.30}$$

$$R_{\{\mu_1\mu_2\}} = A_1 p_{\mu_1} p_{\mu_2} + A_2 g_{\mu_1\mu_2}, \tag{5.31}$$

$$R_{\{\mu_1\mu_2\mu_3\}} = A_1 p_{\mu_1} p_{\mu_2} p_{\mu_3} + A_2 g_{\{\mu_1\mu_2} p_{\mu_3\}}. \tag{5.32}$$

The scalars A_j have in general different mass dimensions. By contracting again with Δ, all trace terms vanish and one obtains

$$I_l(p, m, n_1, \ldots, n_j) = \Delta^{\mu_1} \cdots \Delta^{\mu_N} R_{\{\mu_1 \ldots \mu_N\}} \tag{5.33}$$

$$= A_1 (\Delta \, . \, p)^N \tag{5.34}$$

and thus the coefficient A_1 in Eq. (5.28) gives the desired result. To obtain it, one constructs a different projector, which is made up only of the external momentum p and the metric tensor. By making a general Ansatz for this projector, applying it to Eq. (5.28) and demanding that the result shall be equal to A_1, the coefficients of the different Lorentz structures can be determined. The projector reads

$$\Pi_{\mu_1 \cdots \mu_N} = F(N) \sum_{i=1}^{[N/2]+1} C(i, N) \left(\prod_{l=1}^{[N/2]-i+1} \frac{g_{\mu_{2l-1}\mu_{2l}}}{p^2} \right) \left(\prod_{k=2[N/2]-2i+3}^{N} \frac{p_{\mu_k}}{p^2} \right). \tag{5.35}$$

For the overall pre-factors $F(N)$ and the coefficients $C(i, N)$, one has to distinguish between even and odd values of N,

$$C^{\text{odd}}(k, N) = (-1)^{N/2+k+1/2} \frac{2^{2k-N/2-3/2} \Gamma(N+1) \Gamma(D/2 + N/2 + k - 3/2)}{\Gamma(N/2 - k + 3/2) \Gamma(2k) \Gamma(D/2 + N/2 - 1/2)}, \tag{5.36}$$

$$F^{\text{odd}}(N) = \frac{2^{3/2-N/2} \Gamma(D/2 + 1/2)}{(D-1) \Gamma(N/2 + D/2 - 1)}, \tag{5.37}$$

$$C^{\text{even}}(k, N) = (-1)^{N/2+k+1} \frac{2^{2k-N/2-2} \Gamma(N+1) \Gamma(D/2 + N/2 - 2 + k)}{\Gamma(N/2 - k + 2) \Gamma(2k-1) \Gamma(D/2 + N/2 - 1)}, \tag{5.38}$$

$$F^{\text{even}}(N) = \frac{2^{1-N/2}\Gamma(D/2+1/2)}{(D-1)\Gamma(N/2+D/2-1/2)}. \tag{5.39}$$

The projector obeys the normalization condition

$$\Pi_{\mu_1,\dots,\mu_N} R^{\mu_1,\dots,\mu_N} = A_1, \tag{5.40}$$

which implies

$$\Pi_{\mu_1\cdots\mu_N} p^{\mu_1}\cdots p^{\mu_N} = 1. \tag{5.41}$$

As an example for the above procedure, we consider the case $N = 3$,

$$\Pi_{\mu_1\mu_2\mu_3} = \frac{1}{D-1}\left(-3\frac{g_{\mu_1\mu_2}p_{\mu_3}}{p^4} + (D+2)\frac{p_{\mu_1}p_{\mu_2}p_{\mu 3}}{p^6}\right). \tag{5.42}$$

Applying this term to (5.23) yields

$$\begin{aligned} I_l(p,m,2,1) = {}& \frac{1}{(D-1)p^6}\int\frac{d^Dk_1}{(2\pi)^D}\cdots\int\frac{d^Dk_l}{(2\pi)^D}\big(-2p^2 q_1\,.\,q_2 p\,.\,q_1 \\ & - p^2 q_1^2 p\,.\,q_2 + (D+2)(q_1\,.\,p)^2 q_2\,.\,p\big) f(k_1,\dots,k_l,p,m). \end{aligned} \tag{5.43}$$

It is important to keep p artificially off-shell until the end of the calculation. By construction, the overall result will not contain any term $\propto 1/p^2$, since the integral one starts with cannot contain such a term. Thus, at the end, these terms have to cancel, one can set $p^2 = 0$ and the remaining constant term in p^2 is the desired result.

The above projectors are similar to the harmonic projectors used in the MINCER-program, cf. [65,75]. These are, however, applied to the virtual forward Compton-amplitude to determine the anomalous dimensions and the moments of the massless Wilson coefficients up to 3-loop order.

The calculation was in general performed in Feynman gauge. For the external quark and gluon lines, the projectors (5.15), (5.13) are applied, which requires to include the ghost terms into the calculation. We also performed part of the calculation keeping the gauge parameter in R_ξ-gauges, in particular for the moments $N = 2, 4$ in the singlet case and $N = 1, 2, 3, 4$ in the non-singlet case, yielding agreement with the results being obtained using Feynman-gauge. In addition, for the moments $N = 2, 4$ in the terms with external gluons, we applied the physical projector in Eq. (5.14), which serves as another verification of our results. The computation of the more complicated diagrams was performed on various 32/64 Gb machines using FORM and for part of the calculation TFORM [76], spending about 250 days of computational time.

5.3. Results

We calculated the unrenormalized operator matrix elements treating the 1PI-contributions explicitly. They contribute to $A_{Qg}^{(3)}$, $A_{gg,Q}^{(3)}$ and $A_{qq,Q}^{(3),\mathsf{NS}}$. One obtains the following representations

$$\begin{aligned} \hat{\hat{A}}_{Qg}^{(3)} = {}& \hat{\hat{A}}_{Qg}^{(3),\mathsf{irr}} - \hat{\hat{A}}_{Qg}^{(2),\mathsf{irr}}\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}^2}{\mu^2}\right) - \hat{\hat{A}}_{Qg}^{(1)}\hat{\Pi}^{(2)}\left(0,\frac{\hat{m}^2}{\mu^2}\right) \\ & + \hat{\hat{A}}_{Qg}^{(1)}\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}^2}{\mu^2}\right)\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}^2}{\mu^2}\right), \end{aligned} \tag{5.44}$$

$$\hat{\hat{A}}_{gg,Q}^{(3)} = \hat{\hat{A}}_{gg,Q}^{(3),\mathsf{irr}} - \hat{\Pi}^{(3)}\left(0,\frac{\hat{m}^2}{\mu^2}\right) - \hat{\hat{A}}_{gg,Q}^{(2),\mathsf{irr}}\hat{\Pi}^{(1)}\left(0,\frac{\hat{m}^2}{\mu^2}\right)$$

$$- 2\hat{\hat{A}}_{gg,Q}^{(1)} \hat{\Pi}^{(2)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) + \hat{\hat{A}}_{gg,Q}^{(1)} \hat{\Pi}^{(1)}\left(0, \frac{\hat{m}^2}{\mu^2}\right) \hat{\Pi}^{(1)}\left(0, \frac{\hat{m}^2}{\mu^2}\right), \tag{5.45}$$

$$\hat{\hat{A}}_{qq,Q}^{(3),\mathsf{NS}} = \hat{\hat{A}}_{qq,Q}^{(3),\mathsf{NS,irr}} - \hat{\Sigma}^{(3)}\left(0, \frac{\hat{m}^2}{\mu^2}\right). \tag{5.46}$$

The self-energies are given in Eqs. (4.5), (4.6), (4.7), (4.9). The calculation of the one-particle irreducible 3-loop contributions is performed using MATAD.[10] The amount of moments, which could be calculated, depended on the available computer resources w.r.t. memory and computational time, as well as possible parallelization using TFORM. Increasing the Mellin moment by two demands both a factor of 6–8 larger memory and CPU time. We have calculated the even moments $N = 2, \ldots, 10$ for $A_{Qg}^{(3)}$, $A_{gg,Q}^{(3)}$, and $A_{qg,Q}^{(3)}$, for $A_{Qq}^{(3),\mathsf{PS}}$ up to $N = 12$, and for $A_{qq,Q}^{(3),\mathsf{NS}}$, $A_{qq,Q}^{(3),\mathsf{PS}}$, $A_{gq,Q}^{(3)}$ up to $N = 14$.

(i) Anomalous dimensions:
The pole terms of the unrenormalized OMEs emerging in the calculation agree with the general structure we presented in Eqs. (4.15), (4.24), (4.25), (4.37), (4.38), (4.45), (4.55). Using lower order renormalization coefficients and the constant terms of the 2-loop results, [29,33,35,86], allows to determine the fixed moments of the 2-loop anomalous dimensions and the contributions $\propto T_F$ of the 3-loop anomalous dimensions, cf. Appendix A.2. All our results agree with the results of Refs. [18,19,23,24,79,80]. The anomalous dimensions $\gamma_{qg}^{(2)}$ and $\gamma_{qq}^{(2),\mathsf{PS}}$ are obtained completely. The present calculation is fully independent both in the algorithms and codes compared to Refs. [18,19,23,24,80] and thus provides a stringent check on these results.

(ii) The constant terms $a_{ij}^{(3)}(N)$:
The constant terms in Eq. (3.3) at $O(a_s^3)$, (4.15), (4.24), (4.25), (4.37), (4.38), (4.45), (4.55), are the new contributions to the non-logarithmic part of the 3-loop massive operator matrix elements, which cannot be constructed by other renormalization constants calculated previously. They are given in Appendix A.3. All other contributions to the heavy flavor Wilson coefficients in the region $Q^2 \gg m^2$ are known for general values of N, cf. Sections 2, 4. The functions $a_{ij}^{(3)}(N)$ still contain coefficients $\propto \zeta_2$ and we will see below, under which circumstances these terms will contribute to the heavy flavor contributions to the deep-inelastic structure functions. The constant B_4, (4.10), emerges as in other massive single-scale calculations [81].

(iii) Moments of the constant terms of the 3-loop massive OMEs:
The logarithmic terms of the renormalized 3-loop massive OMEs are determined by known renormalization constants and can be inferred from Eqs. (4.17), (4.26), (4.27), (4.39), (4.40), (4.47), (4.58). In the following, we consider as examples the non-logarithmic contributions to the second moments of the renormalized massive OMEs. We refer to coupling constant renormalization in the $\overline{\mathsf{MS}}$-scheme and compare the results performing the mass renormalization in the on-shell scheme (m) and the $\overline{\mathsf{MS}}$-scheme ($\bar{m}$).

For the matrix elements with external gluons, we obtain:

$$A_{Qg}^{(3),\overline{\mathsf{MS}}}(\mu^2 = m^2, 2)$$

[10] Partial results of the calculation were presented in [77,78].

$$
\begin{aligned}
&= T_F C_A^2\left(\frac{174\,055}{4374} - \frac{88}{9}\mathsf{B}_4 + 72\zeta_4 - \frac{29\,431}{324}\zeta_3\right) \\
&\quad + T_F C_F C_A\left(-\frac{18\,002}{729} + \frac{208}{9}\mathsf{B}_4 - 104\zeta_4 + \frac{2186}{9}\zeta_3 - \frac{64}{3}\zeta_2 + 64\zeta_2\ln(2)\right) \\
&\quad + T_F C_F^2\left(-\frac{8879}{729} - \frac{64}{9}\mathsf{B}_4 + 32\zeta_4 - \frac{701}{81}\zeta_3 + 80\zeta_2 - 128\zeta_2\ln(2)\right) \\
&\quad + T_F^2 C_A\left(-\frac{21\,586}{2187} + \frac{3605}{162}\zeta_3\right) + T_F^2 C_F\left(-\frac{55\,672}{729} + \frac{889}{81}\zeta_3 + \frac{128}{3}\zeta_2\right) \\
&\quad + n_f T_F^2 C_A\left(-\frac{7054}{2187} - \frac{704}{81}\zeta_3\right) + n_f T_F^2 C_F\left(-\frac{22\,526}{729} + \frac{1024}{81}\zeta_3 - \frac{64}{3}\zeta_2\right), \qquad (5.47)
\end{aligned}
$$

$$
\begin{aligned}
&A_{Qg}^{(3),\overline{\mathsf{MS}}}\left(\mu^2 = \bar{m}^2, 2\right) \\
&= T_F C_A^2\left(\frac{174\,055}{4374} - \frac{88}{9}\mathsf{B}_4 + 72\zeta_4 - \frac{29\,431}{324}\zeta_3\right) \\
&\quad + T_F C_F C_A\left(-\frac{123\,113}{729} + \frac{208}{9}\mathsf{B}_4 - 104\zeta_4 + \frac{2330}{9}\zeta_3\right) \\
&\quad + T_F C_F^2\left(-\frac{8042}{729} - \frac{64}{9}\mathsf{B}_4 + 32\zeta_4 - \frac{3293}{81}\zeta_3\right) \\
&\quad + T_F^2 C_A\left(-\frac{21\,586}{2187} + \frac{3605}{162}\zeta_3\right) + T_F^2 C_F\left(-\frac{9340}{729} + \frac{889}{81}\zeta_3\right) \\
&\quad + n_f T_F^2 C_A\left(-\frac{7054}{2187} - \frac{704}{81}\zeta_3\right) + n_f T_F^2 C_F\left(\frac{478}{729} + \frac{1024}{81}\zeta_3\right), \qquad (5.48)
\end{aligned}
$$

$$
\begin{aligned}
&A_{qg,Q}^{(3),\overline{\mathsf{MS}}}\left(\mu^2 = m^2, 2\right) \\
&= n_f T_F^2 C_A\left(\frac{64\,280}{2187} - \frac{704}{81}\zeta_3\right) + n_f T_F^2 C_F\left(-\frac{7382}{729} + \frac{1024}{81}\zeta_3\right), \qquad (5.49)
\end{aligned}
$$

$$
\begin{aligned}
&A_{gg,Q}^{(3),\overline{\mathsf{MS}}}\left(\mu^2 = m^2, 2\right) \\
&= T_F C_A^2\left(-\frac{174\,055}{4374} + \frac{88}{9}\mathsf{B}_4 - 72\zeta_4 + \frac{29\,431}{324}\zeta_3\right) \qquad (5.50) \\
&\quad + T_F C_F C_A\left(\frac{18\,002}{729} - \frac{208}{9}\mathsf{B}_4 + 104\zeta_4 - \frac{2186}{9}\zeta_3 + \frac{64}{3}\zeta_2 - 64\zeta_2\ln(2)\right) \\
&\quad + T_F C_F^2\left(\frac{8879}{729} + \frac{64}{9}\mathsf{B}_4 - 32\zeta_4 + \frac{701}{81}\zeta_3 - 80\zeta_2 + 128\zeta_2\ln(2)\right) \\
&\quad + T_F^2 C_A\left(\frac{21\,586}{2187} - \frac{3605}{162}\zeta_3\right) + T_F^2 C_F\left(\frac{55\,672}{729} - \frac{889}{81}\zeta_3 - \frac{128}{3}\zeta_2\right) \\
&\quad + n_f T_F^2 C_A\left(-\frac{57\,226}{2187} + \frac{1408}{81}\zeta_3\right) + n_f T_F^2 C_F\left(\frac{29\,908}{729} - \frac{2048}{81}\zeta_3 + \frac{64}{3}\zeta_2\right), \qquad (5.51)
\end{aligned}
$$

$$
\begin{aligned}
&A_{gg,Q}^{(3),\overline{\mathsf{MS}}}\left(\mu^2 = \bar{m}^2, 2\right) \\
&= T_F C_A^2\left(-\frac{174\,055}{4374} + \frac{88}{9}\mathsf{B}_4 - 72\zeta_4 + \frac{29\,431}{324}\zeta_3\right)
\end{aligned}
$$

$$+ T_F C_F C_A\left(\frac{123\,113}{729} - \frac{208}{9}\mathsf{B}_4 + 104\zeta_4 - \frac{2330}{9}\zeta_3\right)$$
$$+ T_F C_F^2\left(\frac{8042}{729} + \frac{64}{9}\mathsf{B}_4 - 32\zeta_4 + \frac{3293}{81}\zeta_3\right)$$
$$+ T_F^2 C_A\left(\frac{21\,586}{2187} - \frac{3605}{162}\zeta_3\right) + T_F^2 C_F\left(\frac{9340}{729} - \frac{889}{81}\zeta_3\right)$$
$$+ n_f T_F^2 C_A\left(-\frac{57\,226}{2187} + \frac{1408}{81}\zeta_3\right) + n_f T_F^2 C_F\left(\frac{6904}{729} - \frac{2048}{81}\zeta_3\right). \tag{5.52}$$

Comparing the operator matrix elements in case of the on-shell scheme and $\overline{\mathsf{MS}}$-scheme, one notices that the terms $\ln(2)\zeta_2$, ζ_2 are absent in the latter. The ζ_2 terms, which contribute to $a_{ij}^{(3)}(N)$, are canceled by other contributions through renormalization. Although the present process is massive, this observation resembles the known result that ζ_2-terms do not contribute in space-like massless higher order calculations in even dimensions [82]. This behaviour is found for all calculated moments. In addition, ζ_4-terms occur, which may partly cancel with those in the 3-loop light Wilson coefficients [26]. Note, that Eq. (5.49) is not sensitive to mass renormalization due to the structure of the contributing diagrams.

An additional check is provided by the sum rule [31],

$$A_{Qg}^{(3)}(N=2) + A_{qg,Q}^{(3)}(N=2) + A_{gg,Q}^{(3)}(N=2) = 0, \tag{5.53}$$

which is fulfilled in all renormalization schemes and as well as on the unrenormalized level.

Unlike the operator matrix element with external gluons, the second moments of the quarkonic OMEs emerge for the first time at $O(a_s^2)$. To 3-loop order, the quarkonic OMEs do not contain terms $\propto \zeta_2$. Due to their simpler structure, mass renormalization in the on-shell-scheme does not give rise to terms $\propto \zeta_2$, $\ln(2)\zeta(2)$. Only the rational contribution in the color factor $\propto T_F C_F^2$ turns out to be different and $A_{qq,Q}^{\mathsf{PS},(3)}$, (5.55), is not affected at all. This holds again for all moments we calculated. The non-logarithmic contributions are given by

$$A_{Qq}^{(3),\overline{\mathsf{MS}},\mathsf{PS}}(\mu^2=m^2,2)$$
$$= T_F C_F C_A\left(\frac{830}{2187} + \frac{64}{9}\mathsf{B}_4 - 64\zeta_4 + \frac{1280}{27}\zeta_3\right)$$
$$+ T_F C_F^2\left(\frac{95\,638}{729} - \frac{128}{9}\mathsf{B}_4 + 64\zeta_4 - \frac{9536}{81}\zeta_3\right) + T_F^2 C_F\left(\frac{53\,144}{2187} - \frac{3584}{81}\zeta_3\right)$$
$$+ n_f T_F^2 C_F\left(-\frac{34\,312}{2187} + \frac{1024}{81}\zeta_3\right),$$
$$A_{Qq}^{(3),\overline{\mathsf{MS}},\mathsf{PS}}(\mu^2=\bar{m}^2,2) = T_F C_F C_A\left(\frac{830}{2187} + \frac{64}{9}\mathsf{B}_4 - 64\zeta_4 + \frac{1280}{27}\zeta_3\right)$$
$$+ T_F C_F^2\left(\frac{78\,358}{729} - \frac{128}{9}\mathsf{B}_4 + 64\zeta_4 - \frac{9536}{81}\zeta_3\right)$$
$$+ T_F^2 C_F\left(\frac{53\,144}{2187} - \frac{3584}{81}\zeta_3\right)$$
$$+ n_f T_F^2 C_F\left(-\frac{34\,312}{2187} + \frac{1024}{81}\zeta_3\right), \tag{5.54}$$

$$A_{qq,Q}^{(3),\overline{\mathsf{MS}},\mathsf{PS}}\big(\mu^2=m^2,2\big)=n_fT_F^2C_F\left(-\frac{52\,168}{2187}+\frac{1024}{81}\zeta_3\right), \tag{5.55}$$

$$\begin{aligned}A_{qq,Q}^{(3),\overline{\mathsf{MS}},\mathsf{NS}}\big(\mu^2=m^2,2\big)={}&T_FC_FC_A\left(-\frac{101\,944}{2187}+\frac{64}{9}\mathsf{B}_4-64\zeta_4+\frac{4456}{81}\zeta_3\right)\\&+T_FC_F^2\left(\frac{283\,964}{2187}-\frac{128}{9}\mathsf{B}_4+64\zeta_4-\frac{848}{9}\zeta_3\right)\\&+T_F^2C_F\left(\frac{25\,024}{2187}-\frac{1792}{81}\zeta_3\right)\\&+n_fT_F^2C_F\left(-\frac{46\,336}{2187}+\frac{1024}{81}\zeta_3\right),\end{aligned} \tag{5.56}$$

$$\begin{aligned}A_{qq,Q}^{(3),\overline{\mathsf{MS}},\mathsf{NS}}\big(\mu^2=\bar{m}^2,2\big)={}&T_FC_FC_A\left(-\frac{101\,944}{2187}+\frac{64}{9}\mathsf{B}_4-64\zeta_4+\frac{4456}{81}\zeta_3\right)\\&+T_FC_F^2\left(\frac{201\,020}{2187}-\frac{128}{9}\mathsf{B}_4+64\zeta_4-\frac{848}{9}\zeta_3\right)\\&+T_F^2C_F\left(\frac{25\,024}{2187}-\frac{1792}{81}\zeta_3\right)\\&+n_fT_F^2C_F\left(-\frac{46\,336}{2187}+\frac{1024}{81}\zeta_3\right),\end{aligned} \tag{5.57}$$

$$\begin{aligned}A_{gq,Q}^{(3),\overline{\mathsf{MS}}}\big(\mu^2=m^2,2\big)={}&T_FC_FC_A\left(\frac{101\,114}{2187}-\frac{128}{9}\mathsf{B}_4+128\zeta_4-\frac{8296}{81}\zeta_3\right)\\&+T_FC_F^2\left(-\frac{570\,878}{2187}+\frac{256}{9}\mathsf{B}_4-128\zeta_4+\frac{17\,168}{81}\zeta_3\right)\\&+T_F^2C_F\left(-\frac{26\,056}{729}+\frac{1792}{27}\zeta_3\right)\\&+n_fT_F^2C_F\left(\frac{44\,272}{729}-\frac{1024}{27}\zeta_3\right),\end{aligned} \tag{5.58}$$

$$\begin{aligned}A_{gq,Q}^{(3),\overline{\mathsf{MS}}}\big(\bar{m}^2,2\big)={}&T_FC_FC_A\left(\frac{101\,114}{2187}-\frac{128}{9}\mathsf{B}_4+128\zeta_4-\frac{8296}{81}\zeta_3\right)\\&+T_FC_F^2\left(-\frac{436\,094}{2187}+\frac{256}{9}\mathsf{B}_4-128\zeta_4+\frac{17\,168}{81}\zeta_3\right)\\&+T_F^2C_F\left(-\frac{26\,056}{729}+\frac{1792}{27}\zeta_3\right)\\&+n_fT_F^2C_F\left(\frac{44\,272}{729}-\frac{1024}{27}\zeta_3\right).\end{aligned} \tag{5.59}$$

Finally, the sum rule [31],

$$A_{Qq}^{(3),\mathsf{PS}}(N=2)+A_{qq,Q}^{(3),\mathsf{PS}}(N=2)+A_{qq,Q}^{(3),\mathsf{NS}}(N=2)+A_{gq,Q}^{(3)}(N=2)=0 \tag{5.60}$$

holds on the unrenormalized level, as well as for the renormalized expressions in all schemes considered.

FORM-codes for the constant terms $a_{ij}^{(3)}(N)$, Appendix A.3, and the corresponding moments of the renormalized massive operator matrix elements, both for the mass renormalization carried out in the on-shell- and $\overline{\mathsf{MS}}$-scheme, are attached to this paper and can be obtained upon request. Phenomenological studies of the 3-loop heavy flavor Wilson coefficients in the region $Q^2 \gg m^2$ will be given elsewhere [83].

6. Heavy quark parton densities

In the kinematic region in which the factorization relation (2.5) holds, one may redefine the results obtained in the fixed flavor number scheme, which allows for a partonic description at the level of $(n_f + 1)$ flavors. As before, we consider n_f massless and one heavy quark flavor. Since parton distributions are process independent quantities, we define the parton distributions for $(n_f + 1)$ flavors from the light-flavor parton distribution functions and the massive operator matrix elements for n_f light flavors. Also in case of the structure functions associated to transverse virtual gauge boson polarizations, like $F_2(x, Q^2)$, the factorization (2.5) only occurs far above threshold, $Q^2 \sim 4m^2x/(1-x)$, and at even larger scales for $F_L(x, Q^2)$. The following set of parton densities is obtained, cf. [31]:

$$\begin{aligned} & f_k\big(n_f+1, \mu^2, m^2, N\big) + f_{\bar{k}}\big(n_f+1, \mu^2, m^2, N\big) \\ & \quad = A_{qq,Q}^{\mathrm{NS}}\left(n_f, \frac{\mu^2}{m^2}, N\right) \cdot \big[f_k\big(n_f, \mu^2, N\big) + f_{\bar{k}}\big(n_f, \mu^2, N\big)\big] \\ & \qquad + \tilde{A}_{qq,Q}^{\mathrm{PS}}\left(n_f, \frac{\mu^2}{m^2}, N\right) \cdot \Sigma\big(n_f, \mu^2, N\big) \\ & \qquad + \tilde{A}_{qg,Q}\left(n_f, \frac{\mu^2}{m^2}, N\right) \cdot G\big(n_f, \mu^2, N\big), \end{aligned} \tag{6.1}$$

$$\begin{aligned} & f_Q\big(n_f+1, \mu^2, m^2, N\big) + f_{\bar{Q}}\big(n_f+1, \mu^2, m^2, N\big) \\ & \quad = A_{Qq}^{\mathrm{PS}}\left(n_f, \frac{\mu^2}{m^2}, N\right) \cdot \Sigma\big(n_f, \mu^2, N\big) + A_{Qg}\left(n_f, \frac{\mu^2}{m^2}, N\right) \cdot G\big(n_f, \mu^2, N\big). \end{aligned} \tag{6.2}$$

Here, $f_k(f_{\bar{k}})$ denote the light quark and anti-quark densities, $f_Q(f_{\bar{Q}})$ the heavy quark densities, and G is the gluon density. The flavor singlet, non-singlet and gluon densities for (n_f+1) flavors are given by

$$\begin{aligned} & \Sigma\big(n_f+1, \mu^2, m^2, N\big) \\ & \quad = \left[A_{qq,Q}^{\mathrm{NS}}\left(n_f, \frac{\mu^2}{m^2}, N\right) + n_f \tilde{A}_{qq,Q}^{\mathrm{PS}}\left(n_f, \frac{\mu^2}{m^2}, N\right) \right. \\ & \qquad \left. + A_{Qq}^{\mathrm{PS}}\left(n_f, \frac{\mu^2}{m^2}, N\right)\right] \cdot \Sigma\big(n_f, \mu^2, N\big) \\ & \qquad + \left[n_f \tilde{A}_{qg,Q}\left(n_f, \frac{\mu^2}{m^2}, N\right) + A_{Qg}\left(n_f, \frac{\mu^2}{m^2}, N\right)\right] \cdot G\big(n_f, \mu^2, N\big), \end{aligned} \tag{6.3}$$

$$\begin{aligned} \Delta\big(n_f+1, \mu^2, m^2, N\big) = {} & f_k\big(n_f+1, \mu^2, N\big) + f_{\bar{k}}\big(n_f+1, \mu^2, m^2, N\big) \\ & - \frac{1}{n_f+1} \Sigma\big(n_f+1, \mu^2, m^2, N\big), \end{aligned} \tag{6.4}$$

$$G\big(n_f+1, \mu^2, m^2, N\big) = A_{gq,Q}\left(n_f, \frac{\mu^2}{m^2}, N\right) \cdot \Sigma\big(n_f, \mu^2, N\big)$$

$$+ A_{gg,Q}\left(n_f, \frac{\mu^2}{m^2}, N\right) \cdot G\left(n_f, \mu^2, N\right). \tag{6.5}$$

Note, that the new parton densities depend on the renormalized heavy quark mass m^2. As outlined above, the corresponding relations for the operator matrix elements depend on the mass-renormalization scheme. Furthermore, $m = m(a_s(\mu^2))$. This has to be taken into account in QCD-analyzes, in particular m^2 cannot be chosen constant.

The normalization of the quarkonic and gluonic operators obtained in the light-cone expansion can be chosen arbitrarily. It is, however, convenient to select the relative factor such, that the non-perturbative nucleon-state expectation values, $\Sigma(n_f, \mu^2, N)$ and $G(n_f, \mu^2, N)$, obey

$$\Sigma\left(n_f, \mu^2, N = 2\right) + G\left(n_f, \mu^2, N = 2\right) = 1 \tag{6.6}$$

due to 4-momentum conservation. As a consequence, the OMEs fulfill the relations (5.53), (5.60). The parton densities (6.1)–(6.5) can be applied in other hard-scattering reactions at high energy colliders in kinematic regions where the corresponding power corrections $\propto (m^2/Q^2)^k$, $k \geqslant 1$ can also be safely disregarded.

Conversely, one may extend the kinematic regime for deep-inelastic scattering to define the distribution functions (6.1)–(6.5) upon knowing the power corrections which occur in the heavy flavor Wilson coefficients $\mathsf{H}_i^j(x, Q^2/\mu^2, m^2/\mu^2)$. This is the case up to 2-loop order. We separate both contributions using Eq. (1.8). If one accounts for $\mathsf{H}_i^{j,\mathsf{power}}(x, Q^2/\mu^2, m^2/\mu^2)$ in the fixed flavor number scheme, Eqs. (6.1)–(6.5) are still valid, but they do not necessarily yield the dominant contributions. In the region closer to threshold, the kinematics of heavy quarks is by far not collinear, which is the main reason that a partonic description has to fail. In any case, it is not possible to use the partonic description (6.1)–(6.5) alone for other hard processes in a kinematic domain with significant power corrections.

7. Conclusions

We calculated the 3-loop massive operator matrix elements, which form the heavy flavor Wilson coefficients, (2.11)–(2.15), together with the known massless Wilson coefficients in the region $Q^2 \gg m^2$ due to the factorization theorem (2.5). All but the power-suppressed contributions are obtained in this way. Furthermore, all operator matrix elements needed to derive massive quark-distributions at the 3-loop level were calculated. We presented in detail the renormalization of the massive operator matrix elements, leading to an intermediary representation in a defined MOM-scheme. This is necessary to maintain the partonic description required for the factorization of the heavy flavor Wilson coefficients into OMEs and the light flavor Wilson coefficients. The representation of the heavy flavor Wilson coefficients in the asymptotic region, effectively reached for the structure function $F_2(x, Q^2)$ for $Q^2/m^2 \simeq 10$, is available for general values of N in analytic form, up to the constant parts $a_{ij}^{(3)}(N)$ of the unrenormalized 3-loop OMEs. A number of fixed values of Mellin moments N for these constant parts were calculated, reaching up to $N = 10, 12, 14$, depending on the complexity of the corresponding operator matrix element. Although general methods are available to reconstruct the recurrence formulae for anomalous dimensions and Wilson-coefficients as a function of N by a finite number of moments, [84], the number of moments calculated for $a_{ij}^{(3)}(N)$ is still far too low. Through the renormalization of the massive OMEs, the corresponding moments of the complete 2-loop anomalous dimensions and the T_F-terms of the 3-loop anomalous dimensions are obtained, as are the moments of the complete anomalous dimensions $\gamma_{qq}^{(2),\mathsf{PS}}(N)$ and $\gamma_{qg}^{(2)}(N)$, which agree with the literature.

The results were presented performing the coupling constant renormalization of the OMEs in the $\overline{\mathsf{MS}}$-scheme and the mass renormalization in the on-shell scheme. After a transformation to the $\overline{\mathsf{MS}}$-mass, the ζ_2-terms are canceled completely. Although being a massive calculation, which is indicated by the emergence of the number B_4, the use of the $\overline{\mathsf{MS}}$-scheme moves the structure of the result towards those observed in massless 3-loop calculations.

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Appendix A

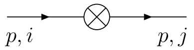
A.1. Feynman rules

For the Feynman rules of QCD, we follow the convention of Ref. [55]. D-dimensional momenta are denoted by p_i and Lorentz indices by Greek letters. Color indices are denoted by $a, b, \ldots$, and i, j are indices of the color matrices. Solid lines represent fermions and curly lines gluons. The Feynman rules for the quarkonic composite operators are given in Fig. 8. Up to $O(g^2)$ they can be found in Refs. [10] and [85]. Note that the $O(g)$ term in the former reference contains a typographical error. We have checked these terms and agree up to normalization factors, which may be partly due to a different convention in the standard Feynman rules. We newly derived the rule with three external gluons. The terms $\gamma_\pm$ refer to the unpolarized $(+)$ and polarized $(-)$ calculation, respectively. Gluon momenta are taken to be incoming. The Feynman rules for the unpolarized gluonic composite operators are given in Fig. 9. Up to $O(g^2)$, they can be found in Refs. [11] and [16]. We have checked these terms and agree up to $O(g^0)$. At $O(g)$, we agree with [11], but not with [16] and [55]. At $O(g^2)$, we do not agree with either of these results, which even differ from each other.[11]

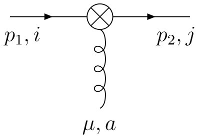
A.2. The 3-loop anomalous dimensions

The 3-loop anomalous dimensions $\gamma_{qq}^{\mathsf{PS}}(N)$ and $\gamma_{qg}(N)$ and the contributions $\propto T_F$ to $\gamma_{qq}^{+,\mathsf{NS}}(N)$, $\gamma_{gq}(N)$ and $\gamma_{gg}(N)$ are obtained from the single pole terms in the present calculation for even values of N and for $\gamma_{qq}^{-,\mathsf{NS}}(N)$ for odd values of N. In the latter case, also $\gamma_{qq}^{s,\mathsf{NS}}(N)$ with $\gamma_{qq}^{v,\mathsf{NS}}(N) = \gamma_{qq}^{-,\mathsf{NS}}(N) + \gamma_{qq}^{s,\mathsf{NS}}(N)$ can be obtained, which will be considered elsewhere [83]. The anomalous dimensions are:

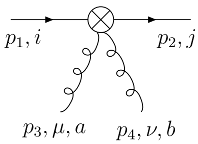
[11] We would like to thank J. Smith for the possibility to compare with their FORM-code used in Refs. [29,56,86,87], to which we agree.



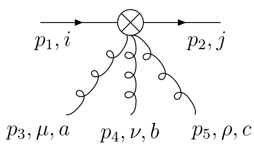
$$\partial^{ij} \not\Delta \gamma_\pm (\Delta . p)^{N-1},\ N \geqslant 1$$



$$g t^a_{ji} \Delta^\mu \not\Delta \gamma_\pm \sum_{j=0}^{N-2} (\Delta . p_1)^j (\Delta . p_2)^{N-j-2},\ N \geqslant 2$$

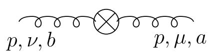


$$g^2 \Delta^\mu \Delta^\nu \not\Delta \gamma_\pm \sum_{j=0}^{N-3} \sum_{l=j+1}^{N-2} (\Delta p_2)^j (\Delta p_1)^{N-l-2}$$
$$\big[(t^a t^b)_{ji} (\Delta p_1 + \Delta p_4)^{l-j-1} + (t^b t^a)_{ji} (\Delta p_1 + \Delta p_3)^{l-j-1}\big],$$
$$N \geqslant 3$$

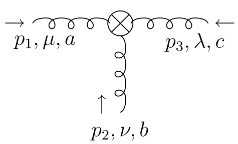


$$g^3 \Delta_\mu \Delta_\nu \Delta_\rho \not\Delta \gamma_\pm \sum_{j=0}^{N-4} \sum_{l=j+1}^{N-3} \sum_{m=l+1}^{N-2} (\Delta . p_2)^j (\Delta . p_1)^{N-m-2}$$
$$\big[(t^a t^b t^c)_{ji} (\Delta . p_4 + \Delta . p_5 + \Delta . p_1)^{l-j-1} (\Delta . p_5 + \Delta . p_1)^{m-l-1}$$
$$+ (t^a t^c t^b)_{ji} (\Delta . p_4 + \Delta . p_5 + \Delta . p_1)^{l-j-1} (\Delta . p_4 + \Delta . p_1)^{m-l-1}$$
$$+ (t^b t^a t^c)_{ji} (\Delta . p_3 + \Delta . p_5 + \Delta . p_1)^{l-j-1} (\Delta . p_5 + \Delta . p_1)^{m-l-1}$$
$$+ (t^b t^c t^a)_{ji} (\Delta . p_3 + \Delta . p_5 + \Delta . p_1)^{l-j-1} (\Delta . p_3 + \Delta . p_1)^{m-l-1}$$
$$+ (t^c t^a t^b)_{ji} (\Delta . p_3 + \Delta . p_4 + \Delta . p_1)^{l-j-1} (\Delta . p_4 + \Delta . p_1)^{m-l-1}$$
$$+ (t^c t^b t^a)_{ji} (\Delta . p_3 + \Delta . p_4 + \Delta . p_1)^{l-j-1} (\Delta . p_3 + \Delta . p_1)^{m-l-1}\big],$$
$$N \geqslant 4$$
$$\gamma_+ = 1,\ \gamma_- = \gamma_5.$$

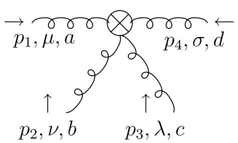
Fig. 8. Feynman rules for quarkonic composite operators. Δ denotes a light-like 4-vector, $\Delta^2 = 0$; N is an integer.



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



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



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

Fig. 9. Feynman rules for gluonic composite operators. Δ denotes a light-like 4-vector, $\Delta^2 = 0$; N is an integer.

(i) $\hat{\gamma}_{qq}^{(2),\mathsf{PS}}(N)$

$$\hat{\gamma}_{qq}^{(2),\mathsf{PS}}(2) = T_F C_F\left[-(1+2n_f)T_F\frac{5024}{243} + \frac{256}{3}(C_F - C_A)\zeta_3 + \frac{10\,136}{243}C_A - \frac{14\,728}{243}C_F\right], \tag{A.1}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{PS}}(4) = T_F C_F\left[-(1+2n_f)T_F\frac{618\,673}{151\,875} + \frac{968}{75}(C_F - C_A)\zeta_3 + \frac{2\,485\,097}{506\,250}C_A - \frac{2\,217\,031}{675\,000}C_F\right], \tag{A.2}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{PS}}(6) = T_F C_F\left[-(1+2n_f)T_F\frac{126\,223\,052}{72\,930\,375} + \frac{3872}{735}(C_F - C_A)\zeta_3 + \frac{1\,988\,624\,681}{4\,084\,101\,000}C_A + \frac{11\,602\,048\,711}{10\,210\,252\,500}C_F\right], \tag{A.3}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{PS}}(8) = T_F C_F\left[-(1+2n_f)T_F\frac{13\,131\,081\,443}{13\,502\,538\,000} + \frac{2738}{945}(C_F - C_A)\zeta_3 - \frac{343\,248\,329\,803}{648\,121\,824\,000}C_A + \frac{39\,929\,737\,384\,469}{22\,684\,263\,840\,000}C_F\right], \tag{A.4}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{PS}}(10) = T_F C_F\left[-(1+2n_f)T_F\frac{265\,847\,305\,072}{420\,260\,754\,375} + \frac{50\,176}{27\,225}(C_F - C_A)\zeta_3 - \frac{1\,028\,766\,412\,107\,043}{1\,294\,403\,123\,475\,000}C_A + \frac{839\,864\,254\,987\,192}{485\,401\,171\,303\,125}C_F\right], \tag{A.5}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{PS}}(12) = T_F C_F\left[-(1+2n_f)T_F\frac{2\,566\,080\,055\,386\,457}{5\,703\,275\,664\,286\,200} + \frac{49\,928}{39\,039}(C_F - C_A)\zeta_3 - \frac{69\,697\,489\,543\,846\,494\,691}{83\,039\,693\,672\,007\,072\,000}C_A + \frac{86\,033\,255\,402\,443\,256\,197}{54\,806\,197\,823\,524\,667\,520}C_F\right]. \tag{A.6}$$

(ii) $\hat{\gamma}_{qg}^{(2)}(N)$

$$\hat{\gamma}_{qg}^{(2)}(2) = T_F\left[(1+2n_f)T_F\left(\frac{8464}{243}C_A - \frac{1384}{243}C_F\right) + \frac{\zeta_3}{3}\left(-416C_AC_F + 288C_A^2 + 128C_F^2\right) - \frac{7178}{81}C_A^2 + \frac{556}{9}C_AC_F - \frac{8620}{243}C_F^2\right], \tag{A.7}$$

$$\hat{\gamma}_{qg}^{(2)}(4) = T_F\left[(1+2n_f)T_F\left(\frac{4\,481\,539}{303\,750}C_A + \frac{9\,613\,841}{3\,037\,500}C_F\right) + \frac{\zeta_3}{25}\left(2832C_A^2 - 3876C_AC_F + 1044C_F^2\right) - \frac{295\,110\,931}{3\,037\,500}C_A^2 + \frac{278\,546\,497}{2\,025\,000}C_AC_F - \frac{757\,117\,001}{12\,150\,000}C_F^2\right], \tag{A.8}$$

$$\hat{\gamma}_{qg}^{(2)}(6) = T_F\bigg[(1+2n_f)T_F\bigg(\frac{86\,617\,163}{11\,668\,860}C_A + \frac{1\,539\,874\,183}{340\,341\,750}C_F\bigg) + \frac{\zeta_3}{735}\big(69\,864C_A^2 - 94\,664C_AC_F + 24\,800C_F^2\big) - \frac{58\,595\,443\,051}{653\,456\,160}C_A^2 + \frac{1\,199\,181\,909\,343}{8\,168\,202\,000}C_AC_F - \frac{2\,933\,980\,223\,981}{40\,841\,010\,000}C_F^2\bigg], \tag{A.9}$$

$$\hat{\gamma}_{qg}^{(2)}(8) = T_F\bigg[(1+2n_f)T_F\bigg(\frac{10\,379\,424\,541}{2\,755\,620\,000}C_A + \frac{7\,903\,297\,846\,481}{1\,620\,304\,560\,000}C_F\bigg) + \zeta_3\bigg(\frac{128\,042}{1575}C_A^2 - \frac{515\,201}{4725}C_AC_F + \frac{749}{27}C_F^2\bigg) - \frac{24\,648\,658\,224\,523}{289\,340\,100\,000}C_A^2 + \frac{4\,896\,295\,442\,015\,177}{32\,406\,091\,200\,000}C_AC_F - \frac{4\,374\,484\,944\,665\,803}{56\,710\,659\,600\,000}C_F^2\bigg], \tag{A.10}$$

$$\hat{\gamma}_{qg}^{(2)}(10) = T_F\bigg[(1+2n_f)T_F\bigg(\frac{1\,669\,885\,489}{988\,267\,500}C_A + \frac{1\,584\,713\,325\,754\,369}{323\,600\,780\,868\,750}C_F\bigg) + \zeta_3\bigg(\frac{1\,935\,952}{27\,225}C_A^2 - \frac{2\,573\,584}{27\,225}C_AC_F + \frac{70\,848}{3025}C_F^2\bigg) - \frac{21\,025\,430\,857\,658\,971}{255\,684\,567\,600\,000}C_A^2 + \frac{926\,990\,216\,580\,622\,991}{6\,040\,547\,909\,550\,000}C_AC_F - \frac{1\,091\,980\,048\,536\,213\,833}{13\,591\,232\,796\,487\,500}C_F^2\bigg]. \tag{A.11}$$

(iii) $\hat{\gamma}_{gq}^{(2)}(N)$

$$\hat{\gamma}_{gq}^{(2)}(2) = T_FC_F\bigg[(1+2n_f)T_F\frac{2272}{81} + \frac{512}{3}(C_A - C_F)\zeta_3 + \frac{88}{9}C_A + \frac{28\,376}{243}C_F\bigg], \tag{A.12}$$

$$\hat{\gamma}_{gq}^{(2)}(4) = T_FC_F\bigg[(1+2n_f)T_F\frac{109\,462}{10\,125} + \frac{704}{15}(C_A - C_F)\zeta_3 - \frac{799}{12\,150}C_A + \frac{14\,606\,684}{759\,375}C_F\bigg], \tag{A.13}$$

$$\hat{\gamma}_{gq}^{(2)}(6) = T_FC_F\bigg[(1+2n_f)T_F\frac{22\,667\,672}{3\,472\,875} + \frac{2816}{105}(C_A - C_F)\zeta_3 - \frac{253\,841\,107}{145\,860\,750}C_A + \frac{20\,157\,323\,311}{2\,552\,563\,125}C_F\bigg], \tag{A.14}$$

$$\hat{\gamma}_{gq}^{(2)}(8) = T_FC_F\bigg[(1+2n_f)T_F\frac{339\,184\,373}{75\,014\,100} + \frac{1184}{63}(C_A - C_F)\zeta_3 - \frac{3\,105\,820\,553}{1\,687\,817\,250}C_A + \frac{8\,498\,139\,408\,671}{2\,268\,426\,384\,000}C_F\bigg], \tag{A.15}$$

$$\hat{\gamma}_{gq}^{(2)}(10) = T_F C_F \bigg[(1+2n_f) T_F \frac{1\,218\,139\,408}{363\,862\,125} + \frac{7168}{495}(C_A - C_F)\zeta_3 - \frac{18\,846\,629\,176\,433}{11\,767\,301\,122\,500} C_A + \frac{529\,979\,902\,254\,031}{323\,600\,780\,868\,750} C_F\bigg], \tag{A.16}$$

$$\hat{\gamma}_{gq}^{(2)}(12) = T_F C_F \bigg[(1+2n_f) T_F \frac{13\,454\,024\,393\,417}{5\,222\,779\,912\,350} + \frac{5056}{429}(C_A - C_F)\zeta_3 - \frac{64\,190\,493\,078\,139\,789}{48\,885\,219\,979\,596\,000} C_A + \frac{1\,401\,404\,001\,326\,440\,151}{3\,495\,293\,228\,541\,114\,000} C_F\bigg], \tag{A.17}$$

$$\hat{\gamma}_{gq}^{(2)}(14) = T_F C_F \bigg[(1+2n_f) T_F \frac{19\,285\,002\,274}{9\,495\,963\,477} + \frac{13\,568}{1365}(C_A - C_F)\zeta_3 - \frac{37\,115\,284\,124\,613\,269}{35\,434\,552\,943\,790\,000} C_A - \frac{40\,163\,401\,444\,446\,690\,479}{104\,797\,690\,331\,258\,925\,000} C_F\bigg]. \tag{A.18}$$

(iv) $\hat{\gamma}_{gg}^{(2)}(N)$

$$\hat{\gamma}_{gg}^{(2)}(2) = T_F \bigg[(1+2n_f) T_F \left(-\frac{8464}{243} C_A + \frac{1384}{243} C_F\right) + \frac{\zeta_3}{3}\left(-288 C_A^2 + 416 C_A C_F - 128 C_F^2\right) + \frac{7178}{81} C_A^2 - \frac{556}{9} C_A C_F + \frac{8620}{243} C_F^2\bigg], \tag{A.19}$$

$$\hat{\gamma}_{gg}^{(2)}(4) = T_F \bigg[(1+2n_f) T_F \left(-\frac{757\,861}{30\,375} C_A - \frac{979\,774}{151\,875} C_F\right) + \frac{\zeta_3}{25}\left(-6264 C_A^2 + 6528 C_A C_F - 264 C_F^2\right) + \frac{53\,797\,499}{607\,500} C_A^2 - \frac{235\,535\,117}{1\,012\,500} C_A C_F + \frac{2\,557\,151}{759\,375} C_F^2\bigg], \tag{A.20}$$

$$\hat{\gamma}_{gg}^{(2)}(6) = T_F \bigg[(1+2n_f) T_F \left(-\frac{52\,781\,896}{2\,083\,725} C_A - \frac{560\,828\,662}{72\,930\,375} C_F\right) + \zeta_3\left(-\frac{75\,168}{245} C_A^2 + \frac{229\,024}{735} C_A C_F - \frac{704}{147} C_F^2\right) + \frac{9\,763\,460\,989}{116\,688\,600} C_A^2 - \frac{9\,691\,228\,129}{32\,672\,808} C_A C_F - \frac{11\,024\,749\,151}{10\,210\,252\,500} C_F^2\bigg], \tag{A.21}$$

$$\hat{\gamma}_{gg}^{(2)}(8) = T_F \bigg[(1+2n_f) T_F \left(-\frac{420\,970\,849}{16\,074\,450} C_A - \frac{6\,990\,254\,812}{843\,908\,625} C_F\right) + \zeta_3\left(-\frac{325\,174}{945} C_A^2 + \frac{327\,764}{945} C_A C_F - \frac{74}{27} C_F^2\right) + \frac{2\,080\,130\,771\,161}{25\,719\,120\,000} C_A^2 - \frac{220\,111\,823\,810\,087}{648\,121\,824\,000} C_A C_F - \frac{14\,058\,417\,959\,723}{5\,671\,065\,960\,000} C_F^2\bigg], \tag{A.22}$$

$$\hat{\gamma}_{gg}^{(2)}(10) = T_F \bigg[(1+2n_f) T_F \left(-\frac{2\,752\,314\,359}{101\,881\,395} C_A - \frac{3\,631\,303\,571\,944}{420\,260\,754\,375} C_F\right)$$

$$+\zeta_3\left(-\frac{70\,985\,968}{190\,575}C_A^2+\frac{71\,324\,656}{190\,575}C_AC_F-\frac{5376}{3025}C_F^2\right)$$
$$+\frac{43\,228\,502\,203\,851\,731}{549\,140\,719\,050\,000}C_A^2$$
$$-\frac{3\,374\,081\,335\,517\,123\,191}{9\,060\,821\,864\,325\,000}C_FC_A$$
$$-\frac{3\,009\,386\,129\,483\,453}{970\,802\,342\,606\,250}C_F^2\Bigg]. \tag{A.23}$$

(v) $\hat{\gamma}_{qq}^{(2),\mathrm{NS},+}(N)$

$$\hat{\gamma}_{qq}^{(2),\mathrm{NS},+}(2)=T_FC_F\Bigg[-(1+2n_f)T_F\frac{1792}{243}+\frac{256}{3}(C_F-C_A)\zeta_3-\frac{12\,512}{243}C_A-\frac{13\,648}{243}C_F\Bigg],$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{NS},+}(4)=T_FC_F\Bigg[-(1+2n_f)T_F\frac{384\,277}{30\,375}+\frac{2512}{15}(C_F-C_A)\zeta_3-\frac{8\,802\,581}{121\,500}C_A-\frac{165\,237\,563}{1\,215\,000}C_F\Bigg], \tag{A.24}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{NS},+}(6)=T_FC_F\Bigg[-(1+2n_f)T_F\frac{160\,695\,142}{10\,418\,625}+\frac{22\,688}{105}(C_F-C_A)\zeta_3-\frac{13\,978\,373}{171\,500}C_A-\frac{44\,644\,018\,231}{243\,101\,250}C_F\Bigg], \tag{A.25}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{NS},+}(8)=T_FC_F\Bigg[-(1+2n_f)T_F\frac{38\,920\,977\,797}{2\,250\,423\,000}+\frac{79\,064}{315}(C_F-C_A)\zeta_3-\frac{1\,578\,915\,745\,223}{18\,003\,384\,000}C_A-\frac{91\,675\,209\,372\,043}{420\,078\,960\,000}C_F\Bigg], \tag{A.26}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{NS},+}(10)=T_FC_F\Bigg[-(1+2n_f)T_F\frac{27\,995\,901\,056\,887}{1\,497\,656\,506\,500}+\frac{192\,880}{693}(C_F-C_A)\zeta_3-\frac{9\,007\,773\,127\,403}{97\,250\,422\,500}C_A-\frac{75\,522\,073\,210\,471\,127}{307\,518\,802\,668\,000}C_F\Bigg], \tag{A.27}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{NS},+}(12)=T_FC_F\Bigg[-(1+2n_f)T_F\frac{65\,155\,853\,387\,858\,071}{3\,290\,351\,344\,780\,500}+\frac{13\,549\,568}{45\,045}(C_F-C_A)\zeta_3-\frac{25\,478\,252\,190\,337\,435\,009}{263\,228\,107\,582\,440\,000}C_A-\frac{35\,346\,062\,280\,941\,906\,036\,867}{131\,745\,667\,845\,011\,220\,000}C_F\Bigg], \tag{A.28}$$

$$\hat{\gamma}_{qq}^{(2),\mathrm{NS},+}(14)=T_FC_F\Bigg[-(1+2n_f)T_F\frac{68\,167\,166\,257\,767\,019}{3\,290\,351\,344\,780\,500}+\frac{2\,881\,936}{9009}(C_F-C_A)\zeta_3-\frac{92\,531\,316\,363\,319\,241\,549}{921\,298\,376\,538\,540\,000}C_A-\frac{37\,908\,544\,797\,975\,614\,512\,733}{131\,745\,667\,845\,011\,220\,000}C_F\Bigg]. \tag{A.29}$$

(vi) $\hat{\gamma}_{qq}^{(2),\mathsf{NS},-}(N)$

$$\hat{\gamma}_{qq}^{(2),\mathsf{NS},-}(1) = 0, \tag{A.30}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{NS},-}(3) = T_F C_F\left[-(1+2n_f)T_F\frac{2569}{243} + \frac{400}{3}(C_F - C_A)\zeta_3 - \frac{62\,249}{972}C_A - \frac{203\,627}{1944}C_F\right], \tag{A.31}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{NS},-}(5) = T_F C_F\left[-(1+2n_f)T_F\frac{431\,242}{30\,375} + \frac{2912}{15}(C_F - C_A)\zeta_3 - \frac{38\,587}{500}C_A - \frac{5\,494\,973}{33\,750}C_F\right], \tag{A.32}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{NS},-}(7) = T_F C_F\left[-(1+2n_f)T_F\frac{1\,369\,936\,511}{83\,349\,000} + \frac{8216}{35}(C_F - C_A)\zeta_3 - \frac{2\,257\,057\,261}{26\,671\,680}C_A - \frac{3\,150\,205\,788\,689}{15\,558\,480\,000}C_F\right], \tag{A.33}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{NS},-}(9) = T_F C_F\left[-(1+2n_f)T_F\frac{20\,297\,329\,837}{1\,125\,211\,500} + \frac{16\,720}{63}(C_F - C_A)\zeta_3 - \frac{126\,810\,403\,414}{1\,406\,514\,375}C_A - \frac{1\,630\,263\,834\,317}{7\,001\,316\,000}C_F\right], \tag{A.34}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{NS},-}(11) = T_F C_F\left[-(1+2n_f)T_F\frac{28\,869\,611\,542\,843}{1\,497\,656\,506\,500} + \frac{1\,005\,056}{3465}(C_F - C_A)\zeta_3 - \frac{1\,031\,510\,572\,686\,647}{10\,892\,047\,320\,000}C_A - \frac{1\,188\,145\,134\,622\,636\,787}{4\,612\,782\,040\,020\,000}C_F\right], \tag{A.35}$$

$$\hat{\gamma}_{qq}^{(2),\mathsf{NS},-}(13) = T_F C_F\left[-(1+2n_f)T_F\frac{66\,727\,681\,292\,862\,571}{3\,290\,351\,344\,780\,500} + \frac{13\,995\,728}{45\,045}(C_F - C_A)\zeta_3 - \frac{90\,849\,626\,920\,977\,361\,109}{921\,298\,376\,538\,540\,000}C_A - \frac{36\,688\,336\,888\,519\,925\,613\,757}{131\,745\,667\,845\,011\,220\,000}C_F\right]. \tag{A.36}$$

We agree with the anomalous dimensions given in [18,19,22–24].

A.3. The $O(\varepsilon^0)$ contributions to $\hat{\hat{A}}_{ij}^{(3)}(N)$

The constant contributions to the unrenormalized massive operator matrix elements at $O(a_s^3)$ read:

(i) $a_{Qq}^{(3),\mathsf{PS}}(N)$

$$a_{Qq}^{(3),\mathsf{PS}}(2) = T_F C_F C_A\left(\frac{117\,290}{2187} + \frac{64}{9}\mathsf{B}_4 - 64\zeta_4 + \frac{1456}{27}\zeta_3 + \frac{224}{81}\zeta_2\right)$$

$$+ T_F C_F^2\left(\frac{42\,458}{243} - \frac{128}{9}\mathsf{B}_4 + 64\zeta_4 - \frac{9664}{81}\zeta_3 + \frac{704}{27}\zeta_2\right)$$
$$+ T_F^2 C_F\left(-\frac{36\,880}{2187} - \frac{4096}{81}\zeta_3 - \frac{736}{81}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(-\frac{76\,408}{2187} + \frac{896}{81}\zeta_3 - \frac{112}{81}\zeta_2\right), \tag{A.37}$$

$$a_{Qq}^{(3),\mathsf{PS}}(4) = T_F C_F C_A\left(\frac{23\,115\,644\,813}{1\,458\,000\,000} + \frac{242}{225}\mathsf{B}_4 - \frac{242}{25}\zeta_4 + \frac{1403}{180}\zeta_3 + \frac{283\,481}{270\,000}\zeta_2\right)$$
$$+ T_F C_F^2\left(-\frac{181\,635\,821\,459}{8\,748\,000\,000} - \frac{484}{225}\mathsf{B}_4 + \frac{242}{25}\zeta_4\right.$$
$$\left. + \frac{577\,729}{40\,500}\zeta_3 + \frac{4\,587\,077}{1\,620\,000}\zeta_2\right)$$
$$+ T_F^2 C_F\left(-\frac{2\,879\,939}{5\,467\,500} - \frac{15\,488}{2025}\zeta_3 - \frac{1118}{2025}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(-\frac{474\,827\,503}{109\,350\,000} + \frac{3388}{2025}\zeta_3 - \frac{851}{20\,250}\zeta_2\right), \tag{A.38}$$

$$a_{Qq}^{(3),\mathsf{PS}}(6) = T_F C_F C_A\left(\frac{111\,932\,846\,538\,053}{10\,291\,934\,520\,000} + \frac{968}{2205}\mathsf{B}_4\right.$$
$$\left. - \frac{968}{245}\zeta_4 + \frac{2\,451\,517}{1\,852\,200}\zeta_3 + \frac{5\,638\,039}{7\,779\,240}\zeta_2\right)$$
$$+ T_F C_F^2\left(-\frac{238\,736\,626\,635\,539}{5\,145\,967\,260\,000} - \frac{1936}{2205}\mathsf{B}_4 + \frac{968}{245}\zeta_4\right.$$
$$\left. + \frac{19\,628\,197}{555\,660}\zeta_3 + \frac{8\,325\,229}{10\,804\,500}\zeta_2\right)$$
$$+ T_F^2 C_F\left(\frac{146\,092\,097}{1\,093\,955\,625} - \frac{61\,952}{19\,845}\zeta_3 - \frac{7592}{99\,225}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(-\frac{82\,616\,977}{45\,378\,900} + \frac{1936}{2835}\zeta_3 - \frac{16\,778}{694\,575}\zeta_2\right), \tag{A.39}$$

$$a_{Qq}^{(3),\mathsf{PS}}(8) = T_F C_F C_A\left(\frac{314\,805\,694\,173\,451\,777}{32\,665\,339\,929\,600\,000} + \frac{1369}{5670}\mathsf{B}_4 - \frac{1369}{630}\zeta_4\right.$$
$$\left. - \frac{202\,221\,853}{137\,168\,640}\zeta_3 + \frac{1\,888\,099\,001}{3\,429\,216\,000}\zeta_2\right)$$
$$+ T_F C_F^2\left(-\frac{25\,652\,839\,216\,168\,097\,959}{457\,314\,759\,014\,400\,000} - \frac{1369}{2835}\mathsf{B}_4 + \frac{1369}{630}\zeta_4\right.$$
$$\left. + \frac{2\,154\,827\,491}{48\,988\,800}\zeta_3 + \frac{12\,144\,008\,761}{48\,009\,024\,000}\zeta_2\right)$$
$$+ T_F^2 C_F\left(\frac{48\,402\,207\,241}{272\,211\,166\,080} - \frac{43\,808}{25\,515}\zeta_3 + \frac{1229}{142\,884}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(-\frac{16\,194\,572\,439\,593}{15\,122\,842\,560\,000} + \frac{1369}{3645}\zeta_3 - \frac{343\,781}{14\,288\,400}\zeta_2\right), \tag{A.40}$$

$$a_{Qq}^{(3),\mathsf{PS}}(10) = T_F C_F C_A\Bigg(\frac{989\,015\,303\,211\,567\,766\,373}{107\,642\,563\,748\,181\,000\,000} + \frac{12\,544}{81\,675}\mathsf{B}_4 - \frac{12\,544}{9075}\zeta_4 - \frac{1\,305\,489\,421}{431\,244\,000}\zeta_3 + \frac{2\,903\,694\,979}{6\,670\,805\,625}\zeta_2\Bigg) + T_F C_F^2\Bigg(-\frac{4\,936\,013\,830\,140\,976\,263\,563}{80\,731\,922\,811\,135\,750\,000} - \frac{25\,088}{81\,675}\mathsf{B}_4 + \frac{12\,544}{9075}\zeta_4 + \frac{94\,499\,430\,133}{1\,940\,598\,000}\zeta_3 + \frac{282\,148\,432}{4\,002\,483\,375}\zeta_2\Bigg) + T_F^2 C_F\Bigg(\frac{430\,570\,223\,624\,411}{2\,780\,024\,890\,190\,625} - \frac{802\,816}{735\,075}\zeta_3 + \frac{319\,072}{11\,026\,125}\zeta_2\Bigg) + n_f T_F^2 C_F\Bigg(-\frac{454\,721\,266\,324\,013}{624\,087\,220\,246\,875} + \frac{175\,616}{735\,075}\zeta_3 - \frac{547\,424}{24\,257\,475}\zeta_2\Bigg), \tag{A.41}$$

$$a_{Qq}^{(3),\mathsf{PS}}(12) = T_F C_F C_A\Bigg(\frac{968\,307\,050\,156\,826\,905\,398\,206\,547}{107\,727\,062\,441\,920\,086\,477\,312\,000} + \frac{12\,482}{117\,117}\mathsf{B}_4 - \frac{12\,482}{13\,013}\zeta_4 - \frac{64\,839\,185\,833\,913}{16\,206\,444\,334\,080}\zeta_3 + \frac{489\,403\,711\,559\,293}{1\,382\,612\,282\,251\,200}\zeta_2\Bigg) + T_F C_F^2\Bigg(-\frac{190\,211\,298\,439\,834\,685\,159\,055\,148\,289}{2\,962\,494\,217\,152\,802\,378\,126\,080\,000} - \frac{24\,964}{117\,117}\mathsf{B}_4 + \frac{12\,482}{13\,013}\zeta_4 + \frac{418\,408\,135\,384\,633}{8\,103\,222\,167\,040}\zeta_3 - \frac{72\,904\,483\,229\,177}{15\,208\,735\,104\,763\,200}\zeta_2\Bigg) + T_F^2 C_F\Bigg(\frac{1\,727\,596\,215\,111\,011\,341}{13\,550\,982\,978\,344\,011\,200} - \frac{798\,848}{1\,054\,053}\zeta_3 + \frac{11\,471\,393}{347\,837\,490}\zeta_2\Bigg) + n_f T_F^2 C_F\Bigg(-\frac{6\,621\,557\,709\,293\,056\,160\,177}{12\,331\,394\,510\,293\,050\,192\,000} + \frac{24\,964}{150\,579}\zeta_3 - \frac{1\,291\,174\,013}{63\,306\,423\,180}\zeta_2\Bigg). \tag{A.42}$$

(ii) $a_{qq,Q}^{(3),\mathsf{PS}}(N)$

$$a_{qq,Q}^{(3),\mathsf{PS}}(2) = n_f T_F^2 C_F\Bigg(-\frac{100\,096}{2187} + \frac{896}{81}\zeta_3 - \frac{256}{81}\zeta_2\Bigg), \tag{A.43}$$

$$a_{qq,Q}^{(3),\mathsf{PS}}(4) = n_f T_F^2 C_F\Bigg(-\frac{118\,992\,563}{21\,870\,000} + \frac{3388}{2025}\zeta_3 - \frac{4739}{20\,250}\zeta_2\Bigg), \tag{A.44}$$

$$a_{qq,Q}^{(3),\mathsf{PS}}(6) = n_f T_F^2 C_F\Bigg(-\frac{17\,732\,294\,117}{10\,210\,252\,500} + \frac{1936}{2835}\zeta_3 - \frac{9794}{694\,575}\zeta_2\Bigg), \tag{A.45}$$

$$a_{qq,Q}^{(3),\mathsf{PS}}(8) = n_f T_F^2 C_F\Bigg(-\frac{20\,110\,404\,913\,057}{27\,221\,116\,608\,000} + \frac{1369}{3645}\zeta_3 + \frac{135\,077}{4\,762\,800}\zeta_2\Bigg), \tag{A.46}$$

$$a_{qq,Q}^{(3),\mathsf{PS}}(10) = n_f T_F^2 C_F \left(-\frac{308\,802\,524\,517\,334}{873\,722\,108\,345\,625} + \frac{175\,616}{735\,075}\zeta_3 + \frac{4\,492\,016}{121\,287\,375}\zeta_2 \right), \tag{A.47}$$

$$a_{qq,Q}^{(3),\mathsf{PS}}(12) = n_f T_F^2 C_F \left(-\frac{6\,724\,380\,801\,633\,998\,071}{38\,535\,607\,844\,665\,781\,850} + \frac{24\,964}{150\,579}\zeta_3 + \frac{583\,767\,694}{15\,826\,605\,795}\zeta_2 \right), \tag{A.48}$$

$$a_{qq,Q}^{(3),\mathsf{PS}}(14) = n_f T_F^2 C_F \left(-\frac{616\,164\,615\,443\,256\,347\,333}{7\,545\,433\,703\,850\,642\,600\,000} + \frac{22\,472}{184\,275}\zeta_3 + \frac{189\,601\,441}{5\,533\,778\,250}\zeta_2 \right). \tag{A.49}$$

(iii) $a_{Qg}^{(3)}(N)$

$$\begin{aligned} a_{Qg}^{(3)}(2) = {} & T_F C_A^2 \left(\frac{170\,227}{4374} - \frac{88}{9}\mathsf{B}_4 + 72\zeta_4 - \frac{31\,367}{324}\zeta_3 + \frac{1076}{81}\zeta_2 \right) \\ & + T_F C_F C_A \left(-\frac{154\,643}{729} + \frac{208}{9}\mathsf{B}_4 - 104\zeta_4 + \frac{7166}{27}\zeta_3 - 54\zeta_2 \right) \\ & + T_F C_F^2 \left(-\frac{15\,574}{243} - \frac{64}{9}\mathsf{B}_4 + 32\zeta_4 - \frac{3421}{81}\zeta_3 + \frac{704}{27}\zeta_2 \right) \\ & + T_F^2 C_A \left(-\frac{20\,542}{2187} + \frac{4837}{162}\zeta_3 - \frac{670}{81}\zeta_2 \right) \\ & + T_F^2 C_F \left(\frac{11\,696}{729} + \frac{569}{81}\zeta_3 + \frac{256}{9}\zeta_2 \right) \\ & - \frac{64}{27} T_F^3 \zeta_3 + n_f T_F^2 C_A \left(-\frac{6706}{2187} - \frac{616}{81}\zeta_3 - \frac{250}{81}\zeta_2 \right) \\ & + n_f T_F^2 C_F \left(\frac{158}{243} + \frac{896}{81}\zeta_3 + \frac{40}{9}\zeta_2 \right), \end{aligned} \tag{A.50}$$

$$\begin{aligned} a_{Qg}^{(3)}(4) = {} & T_F C_A^2 \left(-\frac{425\,013\,969\,083}{2\,916\,000\,000} - \frac{559}{50}\mathsf{B}_4 + \frac{2124}{25}\zeta_4 - \frac{352\,717\,109}{5\,184\,000}\zeta_3 \right. \\ & \left. - \frac{4\,403\,923}{270\,000}\zeta_2 \right) \\ & + T_F C_F C_A \left(-\frac{95\,898\,493\,099}{874\,800\,000} + \frac{646}{25}\mathsf{B}_4 - \frac{2907}{25}\zeta_4 \right. \\ & \left. + \frac{172\,472\,027}{864\,000}\zeta_3 - \frac{923\,197}{40\,500}\zeta_2 \right) \\ & + T_F C_F^2 \left(-\frac{87\,901\,205\,453}{699\,840\,000} - \frac{174}{25}\mathsf{B}_4 + \frac{783}{25}\zeta_4 + \frac{937\,829}{12\,960}\zeta_3 \right. \\ & \left. + \frac{62\,019\,319}{3\,240\,000}\zeta_2 \right) \end{aligned}$$

$$+ T_F^2 C_A \left(\frac{960\,227\,179}{29\,160\,000} + \frac{1\,873\,781}{51\,840}\zeta_3 + \frac{120\,721}{13\,500}\zeta_2 \right)$$
$$+ T_F^2 C_F \left(-\frac{1\,337\,115\,617}{874\,800\,000} + \frac{73\,861}{324\,000}\zeta_3 + \frac{8\,879\,111}{810\,000}\zeta_2 \right)$$
$$- \frac{176}{135} T_F^3 \zeta_3 + n_f T_F^2 C_A \left(\frac{947\,836\,283}{72\,900\,000} - \frac{18\,172}{2025}\zeta_3 - \frac{11\,369}{13\,500}\zeta_2 \right)$$
$$+ n_f T_F^2 C_F \left(\frac{8\,164\,734\,347}{4\,374\,000\,000} + \frac{130\,207}{20\,250}\zeta_3 + \frac{1\,694\,939}{810\,000}\zeta_2 \right), \qquad \text{(A.51)}$$

$$a_{Qg}^{(3)}(6) = T_F C_A^2 \left(-\frac{48\,989\,733\,311\,629\,681}{263\,473\,523\,712\,000} - \frac{2938}{315}\mathsf{B}_4 + \frac{17\,466}{245}\zeta_4 \right.$$
$$\left. - \frac{748\,603\,616\,077}{11\,379\,916\,800}\zeta_3 - \frac{93\,013\,721}{3\,457\,440}\zeta_2 \right)$$
$$+ T_F C_F C_A \left(\frac{712\,876\,107\,019}{55\,319\,040\,000} + \frac{47\,332}{2205}\mathsf{B}_4 - \frac{23\,666}{245}\zeta_4 \right.$$
$$\left. + \frac{276\,158\,927\,731}{1\,896\,652\,800}\zeta_3 + \frac{4\,846\,249}{11\,113\,200}\zeta_2 \right)$$
$$+ T_F C_F^2 \left(-\frac{38\,739\,867\,811\,364\,113}{137\,225\,793\,600\,000} - \frac{2480}{441}\mathsf{B}_4 + \frac{1240}{49}\zeta_4 \right.$$
$$\left. + \frac{148\,514\,798\,653}{711\,244\,800}\zeta_3 + \frac{4\,298\,936\,309}{388\,962\,000}\zeta_2 \right)$$
$$+ T_F^2 C_A \left(\frac{706\,058\,069\,789\,557}{18\,819\,537\,408\,000} + \frac{3\,393\,002\,903}{116\,121\,600}\zeta_3 + \frac{6\,117\,389}{555\,660}\zeta_2 \right)$$
$$+ T_F^2 C_F \left(-\frac{447\,496\,496\,568\,703}{54\,890\,317\,440\,000} - \frac{666\,922\,481}{284\,497\,920}\zeta_3 + \frac{49\,571\,129}{9\,724\,050}\zeta_2 \right)$$
$$- \frac{176}{189} T_F^3 \zeta_3 + n_f T_F^2 C_A \left(\frac{12\,648\,331\,693}{735\,138\,180} - \frac{4433}{567}\zeta_3 + \frac{23\,311}{111\,132}\zeta_2 \right)$$
$$+ n_f T_F^2 C_F \left(-\frac{8\,963\,002\,169\,173}{1\,715\,322\,420\,000} + \frac{111\,848}{19\,845}\zeta_3 + \frac{11\,873\,563}{19\,448\,100}\zeta_2 \right), \qquad \text{(A.52)}$$

$$a_{Qg}^{(3)}(8) = T_F C_A^2 \left(-\frac{358\,497\,428\,780\,844\,484\,961}{2\,389\,236\,291\,993\,600\,000} - \frac{899\,327}{113\,400}\mathsf{B}_4 + \frac{64\,021}{1050}\zeta_4 \right.$$
$$\left. - \frac{12\,321\,174\,818\,444\,641}{112\,368\,549\,888\,000}\zeta_3 - \frac{19\,581\,298\,057}{612\,360\,000}\zeta_2 \right)$$
$$+ T_F C_F C_A \left(\frac{941\,315\,502\,886\,297\,276\,939}{8\,362\,327\,021\,977\,600\,000} \right.$$
$$+ \frac{515\,201}{28\,350}\mathsf{B}_4 - \frac{515\,201}{6300}\zeta_4 + \frac{5\,580\,970\,944\,338\,269}{56\,184\,274\,944\,000}\zeta_3$$
$$\left. + \frac{495\,290\,785\,657}{34\,292\,160\,000}\zeta_2 \right)$$
$$+ T_F C_F^2 \left(-\frac{23\,928\,053\,971\,795\,796\,451\,443}{36\,585\,180\,721\,152\,000\,000} \right.$$

$$
\begin{aligned}
&- \frac{749}{162}\mathsf{B}_4 + \frac{749}{36}\zeta_4 + \frac{719\,875\,828\,314\,061}{1\,404\,606\,873\,600}\zeta_3 \\
&+ \frac{2\,484\,799\,653\,079}{480\,090\,240\,000}\zeta_2\biggr) \\
&+ T_F^2 C_A\biggl(\frac{156\,313\,300\,657\,148\,129}{4\,147\,979\,673\,600\,000} + \frac{58\,802\,880\,439}{2\,388\,787\,200}\zeta_3 \\
&+ \frac{46\,224\,083}{4\,082\,400}\zeta_2\biggr) \\
&+ T_F^2 C_F\biggl(-\frac{986\,505\,627\,362\,913\,047}{87\,107\,573\,145\,600\,000} - \frac{185\,046\,016\,777}{50\,164\,531\,200}\zeta_3 \\
&+ \frac{7\,527\,074\,663}{3\,429\,216\,000}\zeta_2\biggr) - \frac{296}{405}T_F^3\zeta_3 + n_f T_F^2 C_A\biggl(\frac{24\,718\,362\,393\,463}{1\,322\,697\,600\,000} \\
&- \frac{125\,356}{18\,225}\zeta_3 + \frac{2\,118\,187}{2\,916\,000}\zeta_2\biggr) + n_f T_F^2 C_F\biggl(-\frac{291\,376\,419\,801\,571\,603}{32\,665\,339\,929\,600\,000} \\
&+ \frac{887\,741}{174\,960}\zeta_3 - \frac{139\,731\,073}{1\,143\,072\,000}\zeta_2\biggr),
\end{aligned}
\tag{A.53}
$$

$$
\begin{aligned}
a_{Qg}^{(3)}(10) = {} & T_F C_A^2\biggl(\frac{6\,830\,363\,463\,566\,924\,692\,253\,659}{685\,850\,575\,063\,965\,696\,000\,000} - \frac{563\,692}{81\,675}\mathsf{B}_4 + \frac{483\,988}{9075}\zeta_4 \\
&- \frac{103\,652\,031\,822\,049\,723}{415\,451\,499\,724\,800}\zeta_3 - \frac{20\,114\,890\,664\,357}{581\,101\,290\,000}\zeta_2\biggr) \\
&+ T_F C_F C_A\biggl(\frac{872\,201\,479\,486\,471\,797\,889\,957\,487}{2\,992\,802\,509\,370\,032\,128\,000\,000} + \frac{1\,286\,792}{81\,675}\mathsf{B}_4 \\
&- \frac{643\,396}{9075}\zeta_4 - \frac{761\,897\,167\,477\,437\,907}{33\,236\,119\,977\,984\,000}\zeta_3 + \frac{15\,455\,008\,277}{660\,342\,375}\zeta_2\biggr) \\
&+ T_F C_F^2\biggl(-\frac{247\,930\,147\,349\,635\,960\,148\,869\,654\,541}{148\,143\,724\,213\,816\,590\,336\,000\,000} - \frac{11\,808}{3025}\mathsf{B}_4 \\
&+ \frac{53\,136}{3025}\zeta_4 + \frac{9\,636\,017\,147\,214\,304\,991}{7\,122\,025\,709\,568\,000}\zeta_3 + \frac{14\,699\,237\,127\,551}{15\,689\,734\,830\,000}\zeta_2\biggr) \\
&+ T_F^2 C_A\biggl(\frac{23\,231\,189\,758\,106\,199\,645\,229}{633\,397\,356\,480\,430\,080\,000} + \frac{123\,553\,074\,914\,173}{5\,755\,172\,290\,560}\zeta_3 \\
&+ \frac{4\,206\,955\,789}{377\,338\,500}\zeta_2\biggr) \\
&+ T_F^2 C_F\biggl(-\frac{18\,319\,931\,182\,630\,444\,611\,912\,149}{1\,410\,892\,611\,560\,158\,003\,200\,000} \\
&- \frac{502\,987\,059\,528\,463}{113\,048\,027\,136\,000}\zeta_3 + \frac{24\,683\,221\,051}{46\,695\,639\,375}\zeta_2\biggr) \\
&- \frac{896}{1485}T_F^3\zeta_3 + n_f T_F^2 C_A\biggl(\frac{297\,277\,185\,134\,077\,151}{15\,532\,837\,481\,700\,000} - \frac{1\,505\,896}{245\,025}\zeta_3 \\
&+ \frac{189\,965\,849}{188\,669\,250}\zeta_2\biggr) + n_f T_F^2 C_F\biggl(-\frac{1\,178\,560\,772\,273\,339\,822\,317}{107\,642\,563\,748\,181\,000\,000}
\end{aligned}
$$

$$+\frac{62\,292\,104}{13\,476\,375}\zeta_3-\frac{49\,652\,772\,817}{93\,391\,278\,750}\zeta_2\Big). \tag{A.54}$$

(iv) $a_{qg,Q}^{(3)}(N)$

$$\begin{aligned}a_{qg,Q}^{(3)}(2)={}&n_fT_F^2C_A\left(\frac{83\,204}{2187}-\frac{616}{81}\zeta_3+\frac{290}{81}\zeta_2\right)\\&+n_fT_F^2C_F\left(-\frac{5000}{243}+\frac{896}{81}\zeta_3-\frac{4}{3}\zeta_2\right),\end{aligned}\tag{A.55}$$

$$\begin{aligned}a_{qg,Q}^{(3)}(4)={}&n_fT_F^2C_A\left(\frac{835\,586\,311}{14\,580\,000}-\frac{18\,172}{2025}\zeta_3+\frac{71\,899}{13\,500}\zeta_2\right)\\&+n_fT_F^2C_F\left(-\frac{21\,270\,478\,523}{874\,800\,000}+\frac{130\,207}{20\,250}\zeta_3-\frac{1\,401\,259}{810\,000}\zeta_2\right),\end{aligned}\tag{A.56}$$

$$\begin{aligned}a_{qg,Q}^{(3)}(6)={}&n_fT_F^2C_A\left(\frac{277\,835\,781\,053}{5\,881\,105\,440}-\frac{4433}{567}\zeta_3+\frac{2\,368\,823}{555\,660}\zeta_2\right)\\&+n_fT_F^2C_F\left(-\frac{36\,123\,762\,156\,197}{1\,715\,322\,420\,000}+\frac{111\,848}{19\,845}\zeta_3\right.\\&\left.-\frac{26\,095\,211}{19\,448\,100}\zeta_2\right),\end{aligned}\tag{A.57}$$

$$\begin{aligned}a_{qg,Q}^{(3)}(8)={}&n_fT_F^2C_A\left(\frac{157\,327\,027\,056\,457}{3\,968\,092\,800\,000}-\frac{125\,356}{18\,225}\zeta_3+\frac{7\,917\,377}{2\,268\,000}\zeta_2\right)\\&+n_fT_F^2C_F\left(-\frac{201\,046\,808\,090\,490\,443}{10\,888\,446\,643\,200\,000}+\frac{887\,741}{174\,960}\zeta_3\right.\\&\left.-\frac{3\,712\,611\,349}{3\,429\,216\,000}\zeta_2\right),\end{aligned}\tag{A.58}$$

$$\begin{aligned}a_{qg,Q}^{(3)}(10)={}&n_fT_F^2C_A\left(\frac{6\,542\,127\,929\,072\,987}{191\,763\,425\,700\,000}-\frac{1\,505\,896}{245\,025}\zeta_3+\frac{1\,109\,186\,999}{377\,338\,500}\zeta_2\right)\\&+n_fT_F^2C_F\left(-\frac{353\,813\,854\,966\,442\,889\,041}{21\,528\,512\,749\,636\,200\,000}+\frac{62\,292\,104}{13\,476\,375}\zeta_3\right.\\&\left.-\frac{83\,961\,181\,063}{93\,391\,278\,750}\zeta_2\right).\end{aligned}\tag{A.59}$$

(v) $a_{gq,Q}^{(3)}(N)$

$$\begin{aligned}a_{gq,Q}^{(3)}(2)={}&T_FC_FC_A\left(-\frac{126\,034}{2187}-\frac{128}{9}\mathsf{B}_4+128\zeta_4-\frac{9176}{81}\zeta_3-\frac{160}{81}\zeta_2\right)\\&+T_FC_F^2\left(-\frac{741\,578}{2187}+\frac{256}{9}\mathsf{B}_4-128\zeta_4+\frac{17\,296}{81}\zeta_3-\frac{4496}{81}\zeta_2\right)\\&+T_F^2C_F\left(\frac{21\,872}{729}+\frac{2048}{27}\zeta_3+\frac{416}{27}\zeta_2\right)\\&+n_fT_F^2C_F\left(\frac{92\,200}{729}-\frac{896}{27}\zeta_3+\frac{208}{27}\zeta_2\right),\end{aligned}\tag{A.60}$$

$$a_{gq,Q}^{(3)}(4) = T_F C_F C_A\left(-\frac{5\,501\,493\,631}{218\,700\,000} - \frac{176}{45}\mathsf{B}_4 + \frac{176}{5}\zeta_4 - \frac{8258}{405}\zeta_3 + \frac{13\,229}{8100}\zeta_2\right)$$
$$+ T_F C_F^2\left(-\frac{12\,907\,539\,571}{145\,800\,000} + \frac{352}{45}\mathsf{B}_4 - \frac{176}{5}\zeta_4 + \frac{132\,232}{2025}\zeta_3 - \frac{398\,243}{27\,000}\zeta_2\right)$$
$$+ T_F^2 C_F\left(\frac{1\,914\,197}{911\,250} + \frac{2816}{135}\zeta_3 + \frac{1252}{675}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(\frac{50\,305\,997}{1\,822\,500} - \frac{1232}{135}\zeta_3 + \frac{626}{675}\zeta_2\right), \qquad \text{(A.61)}$$

$$a_{gq,Q}^{(3)}(6) = T_F C_F C_A\left(-\frac{384\,762\,916\,141}{24\,504\,606\,000} - \frac{704}{315}\mathsf{B}_4 + \frac{704}{35}\zeta_4 - \frac{240\,092}{19\,845}\zeta_3 + \frac{403\,931}{463\,050}\zeta_2\right)$$
$$+ T_F C_F^2\left(-\frac{40\,601\,579\,774\,533}{918\,922\,725\,000} + \frac{1408}{315}\mathsf{B}_4 - \frac{704}{35}\zeta_4 + \frac{27\,512\,264}{694\,575}\zeta_3 - \frac{24\,558\,841}{3\,472\,875}\zeta_2\right)$$
$$+ T_F^2 C_F\left(-\frac{279\,734\,446}{364\,651\,875} + \frac{11\,264}{945}\zeta_3 + \frac{8816}{33\,075}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(\frac{4\,894\,696\,577}{364\,651\,875} - \frac{704}{135}\zeta_3 + \frac{4408}{33\,075}\zeta_2\right), \qquad \text{(A.62)}$$

$$a_{gq,Q}^{(3)}(8) = T_F C_F C_A\left(-\frac{10\,318\,865\,954\,633\,473}{816\,633\,498\,240\,000} - \frac{296}{189}\mathsf{B}_4 + \frac{296}{21}\zeta_4 - \frac{1\,561\,762}{178\,605}\zeta_3 + \frac{30\,677\,543}{85\,730\,400}\zeta_2\right)$$
$$+ T_F C_F^2\left(-\frac{305\,405\,135\,103\,422\,947}{11\,432\,868\,975\,360\,000} + \frac{592}{189}\mathsf{B}_4 - \frac{296}{21}\zeta_4 + \frac{124\,296\,743}{4\,286\,520}\zeta_3 - \frac{4\,826\,251\,837}{1\,200\,225\,600}\zeta_2\right)$$
$$+ T_F^2 C_F\left(-\frac{864\,658\,160\,833}{567\,106\,596\,000} + \frac{4736}{567}\zeta_3 - \frac{12\,613}{59\,535}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(\frac{9\,330\,164\,983\,967}{1\,134\,213\,192\,000} - \frac{296}{81}\zeta_3 - \frac{12\,613}{119\,070}\zeta_2\right), \qquad \text{(A.63)}$$

$$a_{gq,Q}^{(3)}(10) = T_F C_F C_A\left(-\frac{1\,453\,920\,909\,405\,842\,897}{130\,475\,834\,846\,280\,000} - \frac{1792}{1485}\mathsf{B}_4 + \frac{1792}{165}\zeta_4 - \frac{1\,016\,096}{147\,015}\zeta_3 + \frac{871\,711}{26\,952\,750}\zeta_2\right)$$
$$+ T_F C_F^2\left(-\frac{11\,703\,382\,372\,448\,370\,173}{667\,205\,973\,645\,750\,000} + \frac{3584}{1485}\mathsf{B}_4 - \frac{1792}{165}\zeta_4\right.$$

$$+\frac{62\,282\,416}{2\,695\,275}\zeta_3-\frac{6\,202\,346\,032}{2\,547\,034\,875}\zeta_2\Big)$$
$$+T_F^2C_F\Big(-\frac{1\,346\,754\,066\,466}{756\,469\,357\,875}+\frac{28\,672}{4455}\zeta_3-\frac{297\,472}{735\,075}\zeta_2\Big)$$
$$+n_fT_F^2C_F\Big(\frac{4\,251\,185\,859\,247}{756\,469\,357\,875}-\frac{12\,544}{4455}\zeta_3-\frac{148\,736}{735\,075}\zeta_2\Big), \quad (A.64)$$

$$a_{gq,Q}^{(3)}(12)=T_FC_FC_A\Big(-\frac{1\,515\,875\,996\,003\,174\,876\,943\,331}{147\,976\,734\,123\,516\,602\,304\,000}-\frac{1264}{1287}\mathsf{B}_4$$
$$+\frac{1264}{143}\zeta_4-\frac{999\,900\,989}{173\,918\,745}\zeta_3-\frac{693\,594\,486\,209}{3\,798\,385\,390\,800}\zeta_2\Big)$$
$$+T_FC_F^2\Big(-\frac{48\,679\,935\,129\,017\,185\,612\,582\,919}{4\,069\,360\,188\,396\,706\,563\,360\,000}+\frac{2528}{1287}\mathsf{B}_4$$
$$-\frac{1264}{143}\zeta_4+\frac{43\,693\,776\,149}{2\,260\,943\,685}\zeta_3-\frac{2\,486\,481\,253\,717}{1\,671\,289\,571\,952}\zeta_2\Big)$$
$$+T_F^2C_F\Big(-\frac{2\,105\,210\,836\,073\,143\,063}{1\,129\,248\,581\,528\,667\,600}+\frac{20\,224}{3861}\zeta_3-\frac{28\,514\,494}{57\,972\,915}\zeta_2\Big)$$
$$+n_fT_F^2C_F\Big(\frac{9\,228\,836\,319\,135\,394\,697}{2\,258\,497\,163\,057\,335\,200}-\frac{8848}{3861}\zeta_3$$
$$-\frac{14\,257\,247}{57\,972\,915}\zeta_2\Big), \quad (A.65)$$

$$a_{gq,Q}^{(3)}(14)=T_FC_FC_A\Big(-\frac{1\,918\,253\,569\,538\,142\,572\,718\,209}{199\,199\,449\,781\,656\,964\,640\,000}-\frac{3392}{4095}\mathsf{B}_4+\frac{3392}{455}\zeta_4$$
$$-\frac{2\,735\,193\,382}{553\,377\,825}\zeta_3-\frac{1\,689\,839\,813\,797}{5\,113\,211\,103\,000}\zeta_2\Big)$$
$$+T_FC_F^2\Big(-\frac{143\,797\,180\,510\,035\,170\,802\,620\,917}{17\,429\,951\,855\,894\,984\,406\,000\,000}+\frac{6784}{4095}\mathsf{B}_4-\frac{3392}{455}\zeta_4$$
$$+\frac{12\,917\,466\,836}{774\,728\,955}\zeta_3-\frac{4\,139\,063\,104\,013}{4\,747\,981\,738\,500}\zeta_2\Big)$$
$$+T_F^2C_F\Big(-\frac{337\,392\,441\,268\,078\,561}{179\,653\,183\,425\,015\,300}+\frac{54\,272}{12\,285}\zeta_3-\frac{98\,112\,488}{184\,459\,275}\zeta_2\Big)$$
$$+n_fT_F^2C_F\Big(\frac{222\,188\,365\,726\,202\,803}{71\,861\,273\,370\,006\,120}-\frac{3392}{1755}\zeta_3$$
$$-\frac{49\,056\,244}{184\,459\,275}\zeta_2\Big), \quad (A.66)$$

(vi) $a_{gg,Q}^{(3)}(N)$

$$a_{gg,Q}^{(3)}(2)=T_FC_A^2\Big(-\frac{170\,227}{4374}+\frac{88}{9}\mathsf{B}_4-72\zeta_4+\frac{31\,367}{324}\zeta_3-\frac{1076}{81}\zeta_2\Big)$$
$$+T_FC_FC_A\Big(\frac{154\,643}{729}-\frac{208}{9}\mathsf{B}_4+104\zeta_4-\frac{7166}{27}\zeta_3+54\zeta_2\Big)$$

$$+ T_F C_F^2\left(\frac{15\,574}{243} + \frac{64}{9}\mathsf{B}_4 - 32\zeta_4 + \frac{3421}{81}\zeta_3 - \frac{704}{27}\zeta_2\right)$$
$$+ T_F^2 C_A\left(\frac{20\,542}{2187} - \frac{4837}{162}\zeta_3 + \frac{670}{81}\zeta_2\right)$$
$$+ T_F^2 C_F\left(-\frac{11\,696}{729} - \frac{569}{81}\zeta_3 - \frac{256}{9}\zeta_2\right)$$
$$+ \frac{64}{27}T_F^3\zeta_3 + n_f T_F^2 C_A\left(-\frac{76\,498}{2187} + \frac{1232}{81}\zeta_3 - \frac{40}{81}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(\frac{538}{27} - \frac{1792}{81}\zeta_3 - \frac{28}{9}\zeta_2\right), \tag{A.67}$$

$$a_{gg,Q}^{(3)}(4) = T_F C_A^2\left(\frac{29\,043\,652\,079}{291\,600\,000} + \frac{533}{25}\mathsf{B}_4 - \frac{4698}{25}\zeta_4\right.$$
$$\left. + \frac{610\,035\,727}{2\,592\,000}\zeta_3 + \frac{92\,341}{6750}\zeta_2\right)$$
$$+ T_F C_F C_A\left(\frac{272\,542\,528\,639}{874\,800\,000} - \frac{1088}{25}\mathsf{B}_4 + \frac{4896}{25}\zeta_4\right.$$
$$\left. - \frac{3\,642\,403}{17\,280}\zeta_3 + \frac{73\,274\,237}{810\,000}\zeta_2\right)$$
$$+ T_F C_F^2\left(\frac{41\,753\,961\,371}{1\,749\,600\,000} + \frac{44}{25}\mathsf{B}_4 - \frac{198}{25}\zeta_4\right.$$
$$\left. + \frac{2\,676\,077}{64\,800}\zeta_3 - \frac{4\,587\,077}{1\,620\,000}\zeta_2\right)$$
$$+ T_F^2 C_A\left(-\frac{1\,192\,238\,291}{14\,580\,000} - \frac{2\,134\,741}{25\,920}\zeta_3 - \frac{16\,091}{675}\zeta_2\right)$$
$$+ T_F^2 C_F\left(-\frac{785\,934\,527}{43\,740\,000} - \frac{32\,071}{8100}\zeta_3 - \frac{226\,583}{8100}\zeta_2\right)$$
$$+ \frac{64}{27}T_F^3\zeta_3 + n_f T_F^2 C_A\left(-\frac{271\,955\,197}{1\,822\,500} + \frac{13\,216}{405}\zeta_3 - \frac{6526}{675}\zeta_2\right)$$
$$+ n_f T_F^2 C_F\left(-\frac{465\,904\,519}{27\,337\,500} - \frac{6776}{2025}\zeta_3 - \frac{61\,352}{10\,125}\zeta_2\right), \tag{A.68}$$

$$a_{gg,Q}^{(3)}(6) = T_F C_A^2\left(\frac{37\,541\,473\,421\,359}{448\,084\,224\,000} + \frac{56\,816}{2205}\mathsf{B}_4 - \frac{56\,376}{245}\zeta_4\right.$$
$$\left. + \frac{926\,445\,489\,353}{2\,844\,979\,200}\zeta_3 + \frac{11\,108\,521}{555\,660}\zeta_2\right)$$
$$+ T_F C_F C_A\left(\frac{18\,181\,142\,251\,969\,309}{54\,890\,317\,440\,000} - \frac{114\,512}{2205}\mathsf{B}_4 + \frac{57\,256}{245}\zeta_4\right.$$
$$\left. - \frac{12\,335\,744\,909}{67\,737\,600}\zeta_3 + \frac{94\,031\,857}{864\,360}\zeta_2\right)$$
$$+ T_F C_F^2\left(\frac{16\,053\,159\,907\,363}{635\,304\,600\,000} + \frac{352}{441}\mathsf{B}_4 - \frac{176}{49}\zeta_4\right.$$

$$+\frac{3\,378\,458\,681}{88\,905\,600}\zeta_3-\frac{8\,325\,229}{10\,804\,500}\zeta_2\Big)$$
$$+T_F^2C_A\Big(-\frac{670\,098\,465\,769}{6\,001\,128\,000}-\frac{25\,725\,061}{259\,200}\zeta_3-\frac{96\,697}{2835}\zeta_2\Big)$$
$$+T_F^2C_F\Big(-\frac{8\,892\,517\,283\,287}{490\,092\,120\,000}-\frac{12\,688\,649}{2\,540\,160}\zeta_3-\frac{2\,205\,188}{77\,175}\zeta_2\Big)$$
$$+\frac{64}{27}T_F^3\zeta_3+n_fT_F^2C_A\Big(-\frac{245\,918\,019\,913}{1\,312\,746\,750}+\frac{3224}{81}\zeta_3-\frac{250\,094}{19\,845}\zeta_2\Big)$$
$$+n_fT_F^2C_F\Big(-\frac{71\,886\,272\,797}{3\,403\,417\,500}-\frac{3872}{2835}\zeta_3-\frac{496\,022}{77\,175}\zeta_2\Big),\qquad (A.69)$$

$$a_{gg,Q}^{(3)}(8)=T_FC_A^2\Big(\frac{512\,903\,304\,712\,347\,607}{18\,665\,908\,531\,200\,000}+\frac{108\,823}{3780}\mathsf{B}_4-\frac{162\,587}{630}\zeta_4$$
$$+\frac{2\,735\,007\,975\,361}{6\,502\,809\,600}\zeta_3+\frac{180\,224\,911}{7\,654\,500}\zeta_2\Big)$$
$$+T_FC_FC_A\Big(\frac{13\,489\,584\,043\,443\,319\,991}{43\,553\,786\,572\,800\,000}-\frac{163\,882}{2835}\mathsf{B}_4+\frac{81\,941}{315}\zeta_4$$
$$-\frac{3\,504\,113\,623\,243}{25\,082\,265\,600}\zeta_3+\frac{414\,844\,703\,639}{3\,429\,216\,000}\zeta_2\Big)$$
$$+T_FC_F^2\Big(\frac{5\,990\,127\,272\,073\,225\,467}{228\,657\,379\,507\,200\,000}+\frac{37}{81}\mathsf{B}_4$$
$$-\frac{37}{18}\zeta_4+\frac{3\,222\,019\,505\,879}{87\,787\,929\,600}\zeta_3-\frac{12\,144\,008\,761}{48\,009\,024\,000}\zeta_2\Big)$$
$$+T_F^2C_A\Big(-\frac{16\,278\,325\,750\,483\,243}{124\,439\,390\,208\,000}-\frac{871\,607\,413}{7\,962\,624}\zeta_3-\frac{591\,287}{14\,580}\zeta_2\Big)$$
$$+T_F^2C_F\Big(-\frac{7\,458\,367\,007\,740\,639}{408\,316\,749\,120\,000}-\frac{291\,343\,229}{52\,254\,720}\zeta_3$$
$$-\frac{2\,473\,768\,763}{85\,730\,400}\zeta_2\Big)+\frac{64}{27}T_F^3\zeta_3$$
$$+n_fT_F^2C_A\Big(-\frac{102\,747\,532\,985\,051}{486\,091\,368\,000}+\frac{54\,208}{1215}\zeta_3-\frac{737\,087}{51\,030}\zeta_2\Big)$$
$$+n_fT_F^2C_F\Big(-\frac{1\,145\,917\,332\,616\,927}{51\,039\,593\,640\,000}-\frac{2738}{3645}\zeta_3$$
$$-\frac{70\,128\,089}{10\,716\,300}\zeta_2\Big),\qquad (A.70)$$

$$a_{gg,Q}^{(3)}(10)=T_FC_A^2\Big(-\frac{15\,434\,483\,462\,331\,661\,005\,275\,759}{327\,337\,774\,462\,347\,264\,000\,000}+\frac{17\,788\,828}{571\,725}\mathsf{B}_4$$
$$-\frac{17\,746\,492}{63\,525}\zeta_4+\frac{269\,094\,476\,549\,521\,109}{519\,314\,374\,656\,000}\zeta_3+\frac{1\,444\,408\,720\,649}{55\,468\,759\,500}\zeta_2\Big)$$
$$+T_FC_FC_A\Big(\frac{20\,7095\,356\,146\,239\,371\,087\,405\,921}{771\,581\,896\,946\,961\,408\,000\,000}-\frac{35\,662\,328}{571\,725}\mathsf{B}_4$$

$$+\frac{17\,831\,164}{63\,525}\zeta_4-\frac{3\,288\,460\,968\,359\,099}{37\,093\,883\,904\,000}\zeta_3+\frac{6\,078\,270\,984\,602}{46\,695\,639\,375}\zeta_2\Big)$$
$$+T_FC_F^2\Big(\frac{553\,777\,925\,867\,720\,521\,493\,231}{20\,667\,372\,239\,650\,752\,000\,000}+\frac{896}{3025}\mathsf{B}_4-\frac{4032}{3025}\zeta_4$$
$$+\frac{7\,140\,954\,579\,599}{198\,717\,235\,200}\zeta_3-\frac{282\,148\,432}{4\,002\,483\,375}\zeta_2\Big)$$
$$+T_F^2C_A\Big(-\frac{63\,059\,843\,481\,895\,502\,807}{433\,789\,788\,579\,840\,000}-\frac{85\,188\,238\,297}{729\,907\,200}\zeta_3$$
$$-\frac{33\,330\,316}{735\,075}\zeta_2\Big)$$
$$+T_F^2C_F\Big(-\frac{655\,690\,580\,559\,958\,774\,157}{35\,787\,657\,557\,836\,800\,000}-\frac{71\,350\,574\,183}{12\,043\,468\,800}\zeta_3$$
$$-\frac{3\,517\,889\,264}{121\,287\,375}\zeta_2\Big)$$
$$+\frac{64}{27}T_F^3\zeta_3+n_fT_F^2C_A\Big(-\frac{6\,069\,333\,056\,458\,984}{26\,476\,427\,525\,625}+\frac{215\,128}{4455}\zeta_3$$
$$-\frac{81\,362\,132}{5\,145\,525}\zeta_2\Big)$$
$$+n_fT_F^2C_F\Big(-\frac{100\,698\,363\,899\,844\,296}{4\,368\,610\,541\,728\,125}-\frac{351\,232}{735\,075}\zeta_3$$
$$-\frac{799\,867\,252}{121\,287\,375}\zeta_2\Big). \qquad (A.71)$$

(vii) $a_{qq,Q}^{(3),\mathsf{NS}}(N)$

$$a_{qq,Q}^{(3),\mathsf{NS}}(1)=0, \qquad (A.72)$$

$$a_{qq,Q}^{(3),\mathsf{NS}}(2)=T_FC_FC_A\Big(\frac{8744}{2187}+\frac{64}{9}\mathsf{B}_4-64\zeta_4+\frac{4808}{81}\zeta_3-\frac{64}{81}\zeta_2\Big)$$
$$+T_FC_F^2\Big(\frac{359\,456}{2187}-\frac{128}{9}\mathsf{B}_4+64\zeta_4-\frac{848}{9}\zeta_3+\frac{2384}{81}\zeta_2\Big)$$
$$+T_F^2C_F\Big(-\frac{28\,736}{2187}-\frac{2048}{81}\zeta_3-\frac{512}{81}\zeta_2\Big) \qquad (A.73)$$
$$+n_fT_F^2C_F\Big(-\frac{100\,096}{2187}+\frac{896}{81}\zeta_3-\frac{256}{81}\zeta_2\Big),$$

$$a_{qq,Q}^{(3),\mathsf{NS}}(3)=T_FC_FC_A\Big(\frac{522\,443}{34\,992}+\frac{100}{9}\mathsf{B}_4-100\zeta_4+\frac{15\,637}{162}\zeta_3+\frac{175}{162}\zeta_2\Big)$$
$$+T_FC_F^2\Big(\frac{35\,091\,701}{139\,968}-\frac{200}{9}\mathsf{B}_4+100\zeta_4-\frac{1315}{9}\zeta_3+\frac{29\,035}{648}\zeta_2\Big)$$
$$+T_F^2C_F\Big(-\frac{188\,747}{8748}-\frac{3200}{81}\zeta_3-\frac{830}{81}\zeta_2\Big)$$

$$+ n_f T_F^2 C_F \left(-\frac{1\,271\,507}{17\,496} + \frac{1400}{81}\zeta_3 - \frac{415}{81}\zeta_2 \right), \tag{A.74}$$

$$\begin{aligned}
a_{qq,Q}^{(3),\mathrm{NS}}(4) = {}& T_F C_F C_A \left(\frac{419\,369\,407}{21\,870\,000} + \frac{628}{45}\mathsf{B}_4 - \frac{628}{5}\zeta_4 + \frac{515\,597}{4050}\zeta_3 + \frac{10\,703}{4050}\zeta_2 \right) \\
& + T_F C_F^2 \left(\frac{137\,067\,007\,129}{437\,400\,000} - \frac{1256}{45}\mathsf{B}_4 + \frac{628}{5}\zeta_4 \right. \\
& \left. - \frac{41\,131}{225}\zeta_3 + \frac{4\,526\,303}{81\,000}\zeta_2 \right) \\
& + T_F^2 C_F \left(-\frac{151\,928\,299}{5\,467\,500} - \frac{20\,096}{405}\zeta_3 - \frac{26\,542}{2025}\zeta_2 \right) \\
& + n_f T_F^2 C_F \left(-\frac{1\,006\,358\,899}{10\,935\,000} + \frac{8792}{405}\zeta_3 - \frac{13\,271}{2025}\zeta_2 \right),
\end{aligned} \tag{A.75}$$

$$\begin{aligned}
a_{qq,Q}^{(3),\mathrm{NS}}(5) = {}& T_F C_F C_A \left(\frac{816\,716\,669}{43\,740\,000} + \frac{728}{45}\mathsf{B}_4 - \frac{728}{5}\zeta_4 + \frac{12\,569}{81}\zeta_3 + \frac{16\,103}{4050}\zeta_2 \right) \\
& + T_F C_F^2 \left(\frac{13\,213\,297\,537}{36\,450\,000} - \frac{1456}{45}\mathsf{B}_4 + \frac{728}{5}\zeta_4 \right. \\
& \left. - \frac{142\,678}{675}\zeta_3 + \frac{48\,391}{750}\zeta_2 \right) \\
& + T_F^2 C_F \left(-\frac{9\,943\,403}{303\,750} - \frac{23\,296}{405}\zeta_3 - \frac{31\,132}{2025}\zeta_2 \right) \\
& + n_f T_F^2 C_F \left(-\frac{195\,474\,809}{1\,822\,500} + \frac{10\,192}{405}\zeta_3 - \frac{15\,566}{2025}\zeta_2 \right),
\end{aligned} \tag{A.76}$$

$$\begin{aligned}
a_{qq,Q}^{(3),\mathrm{NS}}(6) = {}& T_F C_F C_A \left(\frac{1\,541\,550\,898\,907}{105\,019\,740\,000} + \frac{5672}{315}\mathsf{B}_4 - \frac{5672}{35}\zeta_4 \right. \\
& \left. + \frac{720\,065}{3969}\zeta_3 + \frac{1\,016\,543}{198\,450}\zeta_2 \right) \\
& + T_F C_F^2 \left(\frac{186\,569\,400\,917}{463\,050\,000} - \frac{11\,344}{315}\mathsf{B}_4 + \frac{5672}{35}\zeta_4 \right. \\
& \left. - \frac{7\,766\,854}{33\,075}\zeta_3 + \frac{55\,284\,811}{771\,750}\zeta_2 \right) \\
& + T_F^2 C_F \left(-\frac{26\,884\,517\,771}{729\,303\,750} - \frac{181\,504}{2835}\zeta_3 - \frac{1\,712\,476}{99\,225}\zeta_2 \right) \\
& + n_f T_F^2 C_F \left(-\frac{524\,427\,335\,513}{4\,375\,822\,500} + \frac{11\,344}{405}\zeta_3 - \frac{856\,238}{99\,225}\zeta_2 \right),
\end{aligned} \tag{A.77}$$

$$\begin{aligned}
a_{qq,Q}^{(3),\mathrm{NS}}(7) = {}& T_F C_F C_A \left(\frac{5\,307\,760\,084\,631}{672\,126\,336\,000} + \frac{2054}{105}\mathsf{B}_4 - \frac{6162}{35}\zeta_4 \right. \\
& \left. + \frac{781\,237}{3780}\zeta_3 + \frac{19\,460\,531}{3\,175\,200}\zeta_2 \right) \\
& + T_F C_F^2 \left(\frac{4\,900\,454\,072\,126\,579}{11\,202\,105\,600\,000} - \frac{4108}{105}\mathsf{B}_4 + \frac{6162}{35}\zeta_4 \right.
\end{aligned}$$

$$
\begin{aligned}
&- \frac{8\,425\,379}{33\,075}\zeta_3 + \frac{1\,918\,429\,937}{24\,696\,000}\zeta_2\Bigg) \\
&+ T_F^2 C_F\Bigg(-\frac{8\,488\,157\,192\,423}{210\,039\,480\,000} - \frac{65\,728}{945}\zeta_3 - \frac{3\,745\,727}{198\,450}\zeta_2\Bigg) \\
&+ n_f T_F^2 C_F\Bigg(-\frac{54\,861\,581\,223\,623}{420\,078\,960\,000} + \frac{4108}{135}\zeta_3 - \frac{3\,745\,727}{396\,900}\zeta_2\Bigg), \qquad \text{(A.78)}
\end{aligned}
$$

$$
\begin{aligned}
a_{qq,Q}^{(3),\mathsf{NS}}(8) = {} & T_F C_F C_A\Bigg(-\frac{37\,259\,291\,367\,883}{38\,887\,309\,440\,000} + \frac{19\,766}{945}\mathsf{B}_4 \\
&- \frac{19\,766}{105}\zeta_4 + \frac{1\,573\,589}{6804}\zeta_3 + \frac{200\,739\,467}{28\,576\,800}\zeta_2\Bigg) \\
&+ T_F C_F^2\Bigg(\frac{3\,817\,101\,976\,847\,353\,531}{8\,166\,334\,982\,400\,000} - \frac{39\,532}{945}\mathsf{B}_4 + \frac{19\,766}{105}\zeta_4 \\
&- \frac{80\,980\,811}{297\,675}\zeta_3 + \frac{497\,748\,102\,211}{6\,001\,128\,000}\zeta_2\Bigg) \\
&+ T_F^2 C_F\Bigg(-\frac{740\,566\,685\,766\,263}{17\,013\,197\,880\,000} - \frac{632\,512}{8505}\zeta_3 - \frac{36\,241\,943}{1\,786\,050}\zeta_2\Bigg) \\
&+ n_f T_F^2 C_F\Bigg(-\frac{4\,763\,338\,626\,853\,463}{34\,026\,395\,760\,000} + \frac{39\,532}{1215}\zeta_3 \\
&- \frac{36\,241\,943}{3\,572\,100}\zeta_2\Bigg), \qquad \text{(A.79)}
\end{aligned}
$$

$$
\begin{aligned}
a_{qq,Q}^{(3),\mathsf{NS}}(9) = {} & T_F C_F C_A\Bigg(-\frac{3\,952\,556\,872\,585\,211}{340\,263\,957\,600\,000} + \frac{4180}{189}\mathsf{B}_4 - \frac{4180}{21}\zeta_4 \\
&+ \frac{21\,723\,277}{85\,050}\zeta_3 + \frac{559\,512\,437}{71\,442\,000}\zeta_2\Bigg) \\
&+ T_F C_F^2\Bigg(\frac{1\,008\,729\,211\,999\,128\,667}{2\,041\,583\,745\,600\,000} - \frac{8360}{189}\mathsf{B}_4 + \frac{4180}{21}\zeta_4 \\
&- \frac{85\,539\,428}{297\,675}\zeta_3 + \frac{131\,421\,660\,271}{1\,500\,282\,000}\zeta_2\Bigg) \\
&+ T_F^2 C_F\Bigg(-\frac{393\,938\,732\,805\,271}{8\,506\,598\,940\,000} - \frac{133\,760}{1701}\zeta_3 - \frac{19\,247\,947}{893\,025}\zeta_2\Bigg) \\
&+ n_f T_F^2 C_F\Bigg(-\frac{2\,523\,586\,499\,054\,071}{17\,013\,197\,880\,000} + \frac{8360}{243}\zeta_3 \\
&- \frac{19\,247\,947}{1\,786\,050}\zeta_2\Bigg), \qquad \text{(A.80)}
\end{aligned}
$$

$$
\begin{aligned}
a_{qq,Q}^{(3),\mathsf{NS}}(10) = {} & T_F C_F C_A\Bigg(-\frac{10\,710\,275\,715\,721\,975\,271}{452\,891\,327\,565\,600\,000} + \frac{48\,220}{2079}\mathsf{B}_4 \\
&- \frac{48\,220}{231}\zeta_4 + \frac{2\,873\,636\,069}{10\,291\,050}\zeta_3 + \frac{961\,673\,201}{112\,266\,000}\zeta_2\Bigg) \\
&+ T_F C_F^2\Bigg(\frac{170\,291\,990\,048\,723\,954\,490\,137}{328\,799\,103\,812\,625\,600\,000} - \frac{96\,440}{2079}\mathsf{B}_4 + \frac{48\,220}{231}\zeta_4
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{10\,844\,970\,868}{36\,018\,675}\zeta_3+\frac{183\,261\,101\,886\,701}{1\,996\,875\,342\,000}\zeta_2\Bigg)\\
&+T_F^2C_F\Bigg(-\frac{6\,080\,478\,350\,275\,977\,191}{124\,545\,115\,080\,540\,000}\\
&-\frac{1\,543\,040}{18\,711}\zeta_3-\frac{2\,451\,995\,507}{108\,056\,025}\zeta_2\Bigg)\\
&+n_fT_F^2C_F\Bigg(-\frac{38\,817\,494\,524\,177\,585\,991}{249\,090\,230\,161\,080\,000}+\frac{96\,440}{2673}\zeta_3\\
&-\frac{2\,451\,995\,507}{216\,112\,050}\zeta_2\Bigg),
\end{aligned}
\tag{A.81}
$$

$$
\begin{aligned}
a_{qq,Q}^{(3),\mathsf{NS}}(11)={}&T_FC_FC_A\Bigg(-\frac{22\,309\,979\,286\,641\,292\,041}{603\,855\,103\,420\,800\,000}+\frac{251\,264}{10\,395}\mathsf{B}_4-\frac{251\,264}{1155}\zeta_4\\
&+\frac{283\,300\,123}{935\,550}\zeta_3+\frac{1\,210\,188\,619}{130\,977\,000}\zeta_2\Bigg)\\
&+T_FC_F^2\Bigg(\frac{177\,435\,748\,292\,579\,058\,982\,241}{328\,799\,103\,812\,625\,600\,000}-\frac{502\,528}{10\,395}\mathsf{B}_4\\
&+\frac{251\,264}{1155}\zeta_4-\frac{451\,739\,191}{1\,440\,747}\zeta_3+\frac{47\,705\,202\,493\,793}{499\,218\,835\,500}\zeta_2\Bigg)\\
&+T_F^2C_F\Bigg(-\frac{6\,365\,809\,346\,912\,279\,423}{124\,545\,115\,080\,540\,000}-\frac{8\,040\,448}{93\,555}\zeta_3\\
&-\frac{512\,808\,781}{21\,611\,205}\zeta_2\Bigg)\\
&+n_fT_F^2C_F\Bigg(-\frac{40\,517\,373\,495\,580\,091\,423}{249\,090\,230\,161\,080\,000}+\frac{502\,528}{13\,365}\zeta_3\\
&-\frac{512\,808\,781}{43\,222\,410}\zeta_2\Bigg),
\end{aligned}
\tag{A.82}
$$

$$
\begin{aligned}
a_{qq,Q}^{(3),\mathsf{NS}}(12)={}&T_FC_FC_A\Bigg(-\frac{126\,207\,343\,604\,156\,227\,942\,043}{2\,463\,815\,086\,971\,638\,400\,000}+\frac{3\,387\,392}{135\,135}\mathsf{B}_4\\
&-\frac{3\,387\,392}{15\,015}\zeta_4+\frac{51\,577\,729\,507}{158\,107\,950}\zeta_3+\frac{2\,401\,246\,832\,561}{243\,486\,243\,000}\zeta_2\Bigg)\\
&+T_FC_F^2\Bigg(\frac{68\,296\,027\,149\,155\,250\,557\,867\,961\,293}{122\,080\,805\,651\,901\,196\,900\,800\,000}-\frac{6\,774\,784}{135\,135}\mathsf{B}_4\\
&+\frac{3\,387\,392}{15\,015}\zeta_4-\frac{79\,117\,185\,295}{243\,486\,243}\zeta_3+\frac{108\,605\,787\,257\,580\,461}{1\,096\,783\,781\,593\,500}\zeta_2\Bigg)\\
&+T_F^2C_F\Bigg(-\frac{189\,306\,988\,923\,316\,881\,320\,303}{3\,557\,133\,031\,815\,302\,940\,000}-\frac{108\,396\,544}{1\,216\,215}\zeta_3\\
&-\frac{90\,143\,221\,429}{3\,652\,293\,645}\zeta_2\Bigg)\\
&+n_fT_F^2C_F\Bigg(-\frac{1\,201\,733\,391\,177\,720\,469\,772\,303}{7\,114\,266\,063\,630\,605\,880\,000}+\frac{6\,774\,784}{173\,745}\zeta_3
\end{aligned}
$$

$$- \frac{90\,143\,221\,429}{7\,304\,587\,290}\zeta_2\bigg), \tag{A.83}$$

$$\begin{aligned}
a_{qq,Q}^{(3),\mathsf{NS}}(13) = {}& T_F C_F C_A\bigg(-\frac{12\,032\,123\,246\,389\,873\,565\,503\,373}{181\,090\,408\,892\,415\,422\,400\,000} + \frac{3\,498\,932}{135\,135}\mathsf{B}_4 \\
& - \frac{3\,498\,932}{15\,015}\zeta_4 + \frac{2\,288\,723\,461}{6\,548\,850}\zeta_3 + \frac{106\,764\,723\,181\,157}{10\,226\,422\,206\,000}\zeta_2\bigg) \\
& + T_F C_F^2\bigg(\frac{10\,076\,195\,142\,551\,036\,234\,891\,679\,659}{17\,440\,115\,093\,128\,742\,414\,400\,000} - \frac{6\,997\,864}{135\,135}\mathsf{B}_4 \\
& + \frac{3\,498\,932}{15\,015}\zeta_4 - \frac{81\,672\,622\,894}{243\,486\,243}\zeta_3 + \frac{448\,416\,864\,235\,277\,759}{4\,387\,135\,126\,374\,000}\zeta_2\bigg) \\
& + T_F^2 C_F\bigg(-\frac{196\,243\,066\,652\,040\,382\,535\,303}{3\,557\,133\,031\,815\,302\,940\,000} - \frac{111\,965\,824}{1\,216\,215}\zeta_3 \\
& - \frac{93\,360\,116\,539}{3\,652\,293\,645}\zeta_2\bigg) \\
& + n_f T_F^2 C_F\bigg(-\frac{1\,242\,840\,812\,874\,342\,588\,467\,303}{7\,114\,266\,063\,630\,605\,880\,000} + \frac{6\,997\,864}{173\,745}\zeta_3 \\
& - \frac{93\,360\,116\,539}{7\,304\,587\,290}\zeta_2\bigg),
\end{aligned} \tag{A.84}$$

$$\begin{aligned}
a_{qq,Q}^{(3),\mathsf{NS}}(14) = {}& T_F C_F C_A\bigg(-\frac{994\,774\,587\,614\,536\,873\,023\,863}{12\,072\,693\,926\,161\,028\,160\,000} + \frac{720\,484}{27\,027}\mathsf{B}_4 \\
& - \frac{720\,484}{3003}\zeta_4 + \frac{6\,345\,068\,237}{17\,027\,010}\zeta_3 + \frac{37\,428\,569\,944\,327}{3\,408\,807\,402\,000}\zeta_2\bigg) \\
& + T_F C_F^2\bigg(\frac{72\,598\,193\,631\,729\,215\,117\,875\,463\,981}{122\,080\,805\,651\,901\,196\,900\,800\,000} - \frac{1\,440\,968}{27\,027}\mathsf{B}_4 \\
& + \frac{720\,484}{3003}\zeta_4 - \frac{2\,101\,051\,892\,878}{6\,087\,156\,075}\zeta_3 + \frac{461\,388\,998\,135\,343\,407}{4\,387\,135\,126\,374\,000}\zeta_2\bigg) \\
& + T_F^2 C_F\bigg(-\frac{40\,540\,032\,063\,650\,894\,708\,251}{711\,426\,606\,363\,060\,588\,000} - \frac{23\,055\,488}{243\,243}\zeta_3 \\
& - \frac{481\,761\,665\,447}{18\,261\,468\,225}\zeta_2\bigg) \\
& + n_f T_F^2 C_F\bigg(-\frac{256\,205\,552\,272\,074\,402\,170\,491}{1\,422\,853\,212\,726\,121\,176\,000} + \frac{1\,440\,968}{34\,749}\zeta_3 \\
& - \frac{481\,761\,665\,447}{36\,522\,936\,450}\zeta_2\bigg).
\end{aligned} \tag{A.85}$$

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