Four-loop wave function renormalization in QCD and QED

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We compute the on-shell wave function renormalization constant to four-loop order in QCD and present numerical results for all coefficients of the $\mathrm{SU}(N_c)$ color factors. We extract the four-loop Heavy Quark Effective Theory anomalous dimension of the heavy-quark field and also discuss the application of our result to QED.

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I. INTRODUCTION

Heavy quarks play an important role in modern particle physics, in particular in the context of QCD. This concerns both virtual effects, the production of massive quarks at collider experiments, and the study of bound state effects of heavy quark–antiquark pairs.

Processes which involve heavy quarks require the renormalization constants for the heavy-quark mass and, when they appear as external particles, also for the quark wave function. The mass renormalization constant in the on-shell scheme, Z_m^{OS}, has been computed to four-loop order in Refs. [1,2]. In this work, we compute the wave function renormalization constant in the on-shell scheme, Z_2^{OS}, to the same order in perturbation theory. Z_2^{OS} is needed for all processes involving external heavy quarks to obtain properly normalized Green's functions as dictated by the Lehmann-Symanzik-Zimmermann reduction formula. Currently, there is no immediate application for the four-loop term of Z_2^{OS}. However, it is an important building block for future applications. For example, it enters all processes which involve the massive four-loop form factor. Z_2^{OS} is also needed for the five-loop corrections to static properties like the anomalous magnetic moment of quarks or, in the case of QED, of leptons.

The calculation of Z_2^{OS} is for several reasons more involved than the one of Z_m^{OS}. First of all, one has to compute the derivative of the fermion self-energy, which leads to higher powers of propagators and thus to a more involved reduction problem. Furthermore, Z_2^{OS} contains both ultraviolet and infrared divergences. Thus, dividing Z_2^{OS} by its $\overline{\mathrm{MS}}$ counterpart does not lead to a finite quantity as in the case of Z_m^{OS}. Z_2^{OS} also depends on the QCD gauge parameter, whereas Z_m^{OS} does not.

The on-shell renormalization constants Z_2^{OS} and Z_m^{OS} can be extracted from the quark propagator by demanding that the quark two-point function has a zero at the position of the on-shell mass and that the residue of the propagator is $-i$. In the following, we briefly sketch the derivation of the relations between the heavy-quark self-energy and Z_2^{OS} and Z_m^{OS}.

The renormalized quark propagator is given by

$$S_F(q) = \frac{-iZ_2^{\mathrm{OS}}}{\not{q} - m^0 + \Sigma(q, M)}, \tag{1}$$

where the renormalization constants are defined as

$$m^0 = Z_m^{\mathrm{OS}} M, \qquad \psi^0 = \sqrt{Z_2^{\mathrm{OS}}}\psi. \tag{2}$$

ψ is the quark field with mass m, M is the on-shell mass, and bare quantities are denoted by a superscript 0. Σ denotes the quark self-energy, which is conveniently decomposed as

$$\Sigma(q, m) = m\Sigma_1(q^2, m) + (\not{q} - m)\Sigma_2(q^2, m). \tag{3}$$

In the limit $q^2 \to M^2$, we require

$$S_F(q) \overset{q^2 \to M^2}{\longrightarrow} \frac{-i}{\not{q} - M}. \tag{4}$$

The calculation outlined in Ref. [3] for the evaluation of $Z_m^{\rm OS}$ and $Z_2^{\rm OS}$ reduces all occurring Feynman diagrams to the evaluation of on-shell integrals at the bare mass scale. In particular, it avoids the introduction of explicit counterterm diagrams. We find it more convenient to follow the more direct approach described in Refs. [4,5], which requires the calculation of diagrams with mass counterterm insertion.

Following Refs. [3–6], we expand Σ around $q^2 = M^2$ and obtain

$$\begin{aligned}\Sigma(q,M) &\approx M\Sigma_1(M^2,M) + (\not{q} - M)\Sigma_2(M^2,M) \\ &\quad + M\frac{\partial}{\partial q^2}\Sigma_1(q^2,M)|_{q^2=M^2}(q^2-M^2) + \cdots \\ &\approx M\Sigma_1(M^2,M) + (\not{q} - M)\left(2M^2\frac{\partial}{\partial q^2}\Sigma_1(q^2,M)|_{q^2=M^2} + \Sigma_2(M^2,M)\right) + \cdots. \end{aligned} \tag{5}$$

Inserting Eq. (5) into Eq. (1) and comparing to Eq. (4) leads to the following formulas for the renormalization constants:

$$\begin{aligned} Z_m^{\rm OS} &= 1 + \Sigma_1(M^2,M), \\ (Z_2^{\rm OS})^{-1} &= 1 + 2M^2\frac{\partial}{\partial q^2}\Sigma_1(q^2,M)|_{q^2=M^2} + \Sigma_2(M^2,M). \end{aligned} \tag{6}$$

Thus, $Z_m^{\rm OS}$ is obtained from Σ_1 for $q^2 = M^2$. To calculate $Z_2^{\rm OS}$, one has to compute the first derivative of the self-energy diagrams. The mass renormalization is taken into account iteratively by calculating lower-loop diagrams with zero-momentum insertions.

It is convenient to introduce $q = Q(1+t)$ with $Q^2 = M^2$ and rewrite the self-energy as

$$\begin{aligned}\Sigma(q,M) &= M\Sigma_1(q^2,M) + (\not{Q} - M)\Sigma_2(q^2,M) \\ &\quad + t\not{Q}\Sigma_2(q^2,M). \end{aligned} \tag{7}$$

Let us now consider the quantity $\mathrm{Tr}\{\frac{\not{Q}+M}{4M^2}\Sigma\}$ and expand it to first order in t, which leads to

$$\begin{aligned}\mathrm{Tr}\left\{\frac{\not{Q}+M}{4M^2}\Sigma(q,M)\right\} &= \Sigma_1(q^2,M) + t\Sigma_2(q^2,M) \\ &= \Sigma_1(M^2,M) + \left(2M^2\frac{\partial}{\partial q^2}\Sigma_1(q^2,M)|_{q^2=M^2} + \Sigma_2(M^2,M)\right)t + \mathcal{O}(t^2). \end{aligned} \tag{8}$$

The comparison to Eq. (6) shows that the leading term provides $Z_m^{\rm OS}$ and the coefficient of the linear term in t leads to $Z_2^{\rm OS}$.

In the next section, we present results for $Z_2^{\rm OS}$ up to four loops, and in Sec. III, we discuss consistency checks which are obtained from matching full QCD to Heavy Quark Effective Theory (HQET). Section IV contains a brief summary and our conclusions.

II. RESULTS FOR $Z_2^{\rm OS}$

The wave function renormalization constant is conveniently cast into the form

$$Z_2^{\rm OS} = 1 + \sum_{j\geq 1}\left(\frac{\alpha_s^0(\mu)}{\pi}\right)^j\left(\frac{e^{\gamma_E}}{4\pi}\right)^{-j\epsilon}\left(\frac{\mu^2}{M^2}\right)^{j\epsilon}\delta Z_2^{(j)}, \tag{9}$$

where the bare strong coupling constant α_s^0 has been used for the parametrization. Note that $\delta Z_2^{(i)}$ for $i \geq 3$ depend on the bare QCD gauge parameter ξ, which is introduced in the gluon propagator via

$$D_g^{\mu\nu}(q) = -i\frac{g^{\mu\nu} - \xi\frac{q^\mu q^\nu}{q^2}}{q^2 + i\varepsilon}. \tag{10}$$

With these choices, we can define the coefficients $\delta Z_2^{(i)}$ such that they do not contain $\log(\mu^2/M^2)$ terms. In fact, they can be combined with the factors $(\mu^2/M^2)^{j\epsilon}$ where j is the loop order [cf. Eq. (9)]. The renormalization of α_s and $(\xi - 1)$ is multiplicative so that, if required, α_s^0 and ξ^0 can be replaced in a straightforward way by their renormalized counterparts using the relations

$$\begin{aligned}\alpha_s^0 &= (\mu^2)^{2\epsilon}Z_{\alpha_s}\alpha_s, \\ \xi^0 - 1 &= Z_3(\xi - 1), \end{aligned} \tag{11}$$

where

$$Z_{\alpha_s} = 1 + \frac{1}{\epsilon}\left(\frac{n_f}{6} - \frac{11}{12}C_A\right)\frac{\alpha_s}{\pi} + \cdots,$$

$$Z_3 = 1 + \frac{1}{\epsilon}\left[-\frac{n_f}{6} + \left(\frac{5}{12} + \frac{1}{8}\xi\right)C_A\right]\frac{\alpha_s}{\pi} + \cdots. \quad (12)$$

$C_A = 3$ is a SU(3) color factor, and n_f is the number of active quarks. The ellipses denote higher-order terms in α_s. To obtain the ultraviolet-renormalized version of $Z_2^{\rm OS}$, we need Z_{α_s} to three loops and Z_3 to one-loop order. Note that in Eq. (9) it is assumed that the heavy-quark mass is renormalized on shell; i.e., all mass renormalization counterterms from lower-order diagrams are included.

For the calculation of the four-loop diagrams, we proceeded in the same way as for the calculation of the mass renormalization constant [1,2] and the muon anomalous magnetic moment [7] and thus refer to Ref. [2] for more details. Let us still describe some complications. After a tensor reduction, we obtain Feynman integrals from the same hundred families with 14 indices as in Refs. [1,2]. The maximal number of positive indices is 11. One can describe the complexity of integrals of a given sector (determined by a decomposition of the set of indices into subsets of positive and nonpositive indices) by the number $\sum|a_i - n_i|$, where the index $n_i = 1$ or 0 characterizes a given sector. What is most crucial for the feasibility of an integration-by-parts (IBP) reduction is the complexity of input integrals in the top sector, i.e., with $n_i = 1$ for $i = 1, 2, \ldots, 11$ and $n_i = 0$ for $i = 12$, 13, 14. In the present calculation, this number was up to 6, while in our previous calculation it was 5. Therefore, the reduction procedure performed with FIRE [8–10] coupled with LiteRed [11,12] and Crusher [13] was essentially more complicated as compared to that of Refs. [1,2].

As in Refs. [1,2], we revealed additional relations between master integrals of different families using symmetries and applied the code TSORT, which is part of the latest FIRE version [10]. In most cases, the master integrals were computed numerically with the help of FIESTA [14–16]. For some master integrals, we used analytic results obtained by a straightforward loop-by-loop integration at general dimension d and also used analytical results obtained for the 13 nontrivial four-loop on-shell master integrals computed in Ref. [17]. As is described in detail in Ref. [2], we also applied Mellin-Barnes representations [18–21]. In the case of one-fold Mellin-Barnes representations, it is possible to obtain a very high precision (up to 1000 digits) so that analytic results can be recovered using the PSLQ algorithm [22]. Often the two-, three-, and higher-fold Mellin-Barnes representations provide a better precision than FIESTA. Recently, a subset of the master integrals has been calculated either analytically or with high numerical precision, in the context of the anomalous magnetic moment of the electron [23]. However, these results are not available to us.

The more complicated IBP reduction resulted in higher ϵ poles in the coefficients of some of the master integrals, so that the corresponding results are needed to higher powers in ϵ. Depending on the integral, we either straightforwardly evaluated more terms with FIESTA or obtained more analytical terms or more numerical terms via Mellin-Barnes integrals.

Let us mention that we compute the self-energies on the right-hand side of Eq. (6) including terms of order ξ^2. We did not evaluate the ξ^3, ξ^4, and ξ^5 contributions. Some diagrams develop ξ^6 terms, which we reduced to master integrals, and we could show that their contributions to $Z_2^{\rm OS}$ add up to zero. Thus, our final result for $Z_2^{\rm OS}$ contains ξ^2 terms. We cannot exclude that also higher-order ξ terms are present but we do not expect that there are ξ^n terms present in $Z_2^{\rm OS}$ for $n \geq 4$.

Let us in a first step turn to the one-, two-, and three-loop results for $Z_2^{\rm OS}$, which are available from Refs. [5,6,24]. We have added higher-order ϵ terms, which are necessary to obtain $Z_2^{\rm OS}$ at four loops. In Appendix B, we present results which in particular include the $\mathcal{O}(\epsilon)$ terms of the three-loop coefficient.

In the following, we present results for all 23 SU(N_c) color structures which occur at four-loop order. It is convenient to decompose $\delta Z_2^{(4)}$ as

$$\begin{aligned}
\delta Z_2^{(4)} = {}& C_F^4\delta Z_2^{FFFF} + C_F^3 C_A\delta Z_2^{FFFA} + C_F^2 C_A^2\delta Z_2^{FFAA} + C_F C_A^3\delta Z_2^{FAAA} \\
& + \frac{d_F^{abcd}d_A^{abcd}}{N_c}\delta Z_2^{d_{FA}} + n_l\frac{d_F^{abcd}d_F^{abcd}}{N_c}\delta Z_2^{d_{FF}L} + n_h\frac{d_F^{abcd}d_F^{abcd}}{N_c}\delta Z_2^{d_{FF}H} \\
& + C_F^3 T n_l\delta Z_2^{FFFL} + C_F^2 C_A T n_l\delta Z_2^{FFAL} + C_F C_A^2 T n_l\delta Z_2^{FAAL} \\
& + C_F^2 T^2 n_l^2\delta Z_2^{FFLL} + C_F C_A T^2 n_l^2\delta Z_2^{FALL} + C_F T^3 n_l^3\delta Z_2^{FLLL} \\
& + C_F^3 T n_h\delta Z_2^{FFFH} + C_F^2 C_A T n_h\delta Z_2^{FFAH} + C_F C_A^2 T n_h\delta Z_2^{FAAH} \\
& + C_F^2 T^2 n_h^2\delta Z_2^{FFHH} + C_F C_A T^2 n_h^2\delta Z_2^{FAHH} + C_F T^3 n_h^3\delta Z_2^{FHHH} \\
& + C_F^2 T^2 n_l n_h\delta Z_2^{FFLH} + C_F C_A T^2 n_l n_h\delta Z_2^{FALH} + C_F T^3 n_l^2 n_h\delta Z_2^{FLLH} \\
& + C_F T^3 n_l n_h^2\delta Z_2^{FLHH},
\end{aligned} \quad (13)$$

where C_F, C_A, T, n_l, and n_h are defined after Eq. (B3) in Appendix B. The new color factors at four loops are the symmetrized traces of four generators in the fundamental and adjoint representation denoted by d_F^{abcd} and d_A^{abcd}, respectively.

In Tables V, VI, VII, and VIII (see Appendix A), we show the numerical results for the coefficients introduced in Eq. (13). The numerical uncertainties have been obtained by adding the uncertainties from each individual master integral in quadrature and multiplying the result by a security factor 10. This approach is quite conservative; however, we observed that there are rare cases where the uncertainty from numerical integration is underestimated by several standard deviations. A factor 10 covers all cases which we have experienced (see also the discussion in Ref. [2]). All coefficients which have a nonzero numerical uncertainty are truncated in such a way that two digits of the uncertainty are shown; otherwise, we present (at least) five significant digits. Note that the n_l^3 and n_l^2 terms are known analytically [17]. None of the other coefficients is known analytically to us, although for some of them, the uncertainty is very small; see, e.g., $C_F n_h^3$.

Let us start with the discussion of Table V. Most of the coefficients are known with an uncertainty of a few percent or below. An exception is the C_F^4 and $C_F^3 C_A$ color factors, where the uncertainty is about 30%. In the case of $n_h(d_F^{abcd})^2$, the uncertainty is larger than the central value, and we are not able to decide whether the corresponding coefficient is zero or numerically small. For some color structures, our precision is below a per mille level, in particular for the most non-Abelian color factor $C_F C_A^3$, which provides the numerically largest contribution.

There are some coefficients in the pole parts where the numerical uncertainty is larger than the central value. In these cases, no definite conclusion can be drawn. Within our (conservative) uncertainty estimate, the results are compatible with zero. Still, in these cases, we cannot exclude a small nonzero result. Note, however, that in most cases the uncertainty is much smaller than the central value. In particular, all color structures except those involving d_F^{abcd} or d_A^{abcd} have a nonzero $1/\epsilon^4$ pole. In fact, we expect that the color structures involving d_F^{abcd} and d_A^{abcd} only have a $1/\epsilon$ pole, which is consistent with our result.

The coefficients in Table VI representing the linear ξ terms are in general much smaller than for $\xi = 0$, and the situation is similar as for the pole terms of Table V: we can conclude that the color structures $C_F^2 C_A^2$, $C_F C_A^3$, $d_F^{abcd} d_A^{abcd}$, $C_F C_A^2 n_l$, $C_F^2 C_A n_h$, $C_F C_A^2 n_h$, $C_F C_A n_h^2$, and $C_F C_A n_l n_h$ have nonzero coefficients. Within our precision, the coefficient of $C_F^3 C_A$ is zero; the central value is of order 10^{-4} and furthermore ten times smaller than the uncertainty. However, a closer look into this contribution shows that nontrivial master integrals are involved, which combine to the numerical result given in Table VI. Since the master integrals are linear independent and since they are beyond "three-loop complexity" (i.e., they are neither products of lower-loop integrals nor contain simple one-loop insertions), we would expect a nonzero coefficient unless there are accidental cancellations. Note that at three-loop order there are two color structures which have ξ-dependent coefficients: $C_F C_A^2$ and $C_F C_A n_h$.

In Table VII, which contains the ξ^2 terms, there are nonzero coefficients for the color structures $C_F C_A^3$, $d_F^{abcd} d_A^{abcd}$, and $C_F C_A^2 n_h$.

It is interesting to check the cancellations between the bare four-loop expression and the mass counterterm contributions (which are known analytically and can be found in the ancillary file for this paper [25]). For this reason, we show in Table VIII the bare four-loop coefficients. The comparison with the corresponding entries in Table V shows that the coefficients of some of the color structures suffer from large cancellations, which in some cases is even more than 2 orders of magnitude (see, e.g., the $C_F^3 n_l$ term). Note that the numerically dominant color structure $C_F C_A^3$ is not affected by mass renormalization.

In Ref. [26], the pole of the color structure $n_l(d_F^{abcd})^2$ has been determined from the requirement that a certain combination of renormalization constants in full QCD and HQET are finite (see also the discussion in Sec. III below). Its analytic expression in our notation reads

$$\delta Z_2^{d_{FF}L} = -\frac{1}{\epsilon}\left(\frac{1}{8} + \frac{\pi^2}{12} - \frac{\zeta_3}{8} - \frac{\pi^2\zeta_3}{12} + \frac{5\zeta_5}{32}\right) + \cdots$$
$$\approx \frac{0.029\,422\,3}{\epsilon} + \cdots, \tag{14}$$

which has to be compared to our numerical result $(0.011 \pm 0.064)/\epsilon + \cdots$ (see Table V). The result in Eq. (14) agrees with our result within the uncertainty. Note, however, that the absolute value of this contribution is quite small, which explains our large relative uncertainty.

It is interesting to insert the numerical values of the color factors and evaluate $\delta Z_2^{(4)}$ for $N_c = 3$. To obtain the corresponding expression, we choose $N_c = 3$ after inserting the master integrals but before combining the uncertainties from the various ϵ expansion coefficients of the color factors. The results for the various powers of n_l are given in Table I. Note that for $\xi = 0$ (top) all uncertainties are of order 10^{-4}. Furthermore, for all powers of n_l, we observe nonzero coefficients in the poles up to fourth order. For completeness, we present in Table I also results for the ξ^1 and ξ^2 terms. For the linear ξ coefficients, we observe nonzero entries only for the n_l^0 and the linear-n_l term. The coefficients of ξ^2 are only nonzero for the n_l^0 contribution.

TABLE I. Results for the coefficients of $\delta Z_2^{(4)}$ after choosing $N_c = 3$. The $\xi = 0$, ξ^1, and ξ^2 contributions are shown in the top, middle, and bottom tables. A security factor 10 has been applied to the uncertainties.

$\xi = 0$	$1/\epsilon^4$	$1/\epsilon^3$	$1/\epsilon^2$	$1/\epsilon$	ϵ^0
n_l^0	$-1.772\,42 \pm 0.000\,40$	-27.6674 ± 0.0041	-317.093 ± 0.029	-3142.15 ± 0.33	$-28\,709.9 \pm 3.2$
n_l^1	$0.460\,936 \pm 0.000\,016$	$6.691\,43 \pm 0.000\,23$	74.6540 ± 0.0013	696.6612 ± 0.0076	6174.290 ± 0.084
n_l^2	$-0.039\,931$	$-0.515\,72$	-5.5055	-48.777	-418.93
n_l^3	$0.001\,157\,41$	$0.012\,538\,6$	$0.126\,757$	$1.071\,05$	8.9160

ξ^1	$1/\epsilon^4$	$1/\epsilon^3$	$1/\epsilon^2$	$1/\epsilon$	ϵ^0
n_l^0	$-0.018\,555 \pm 0.000\,011$	$0.034\,239 \pm 0.000\,089$	$-0.056\,78 \pm 0.000\,52$	5.2230 ± 0.0028	36.820 ± 0.017
n_l^1	$0.001\,736\,11$	$-0.005\,208\,3$	$0.022\,426\,9$	$-0.348\,63$	$-1.611\,05$

ξ^2	$1/\epsilon^4$	$1/\epsilon^3$	$1/\epsilon^2$	$1/\epsilon$	ϵ^0
n_l^0	$0.000\,000\,2 \pm 0.000\,003\,8$	$0.001\,952 \pm 0.000\,026$	$-0.030\,22 \pm 0.000\,12$	$-0.186\,86 \pm 0.000\,61$	-2.9266 ± 0.0028

TABLE II. Results for $Z_2^{\rm OS}$ specified to QED.

	$1/\epsilon^4$	$1/\epsilon^3$	$1/\epsilon^2$	$1/\epsilon$	ϵ^0
n_l^0	$0.205\,00 \pm 0.000\,37$	0.5980 ± 0.0027	-0.895 ± 0.021	-6.18 ± 0.17	-17.4 ± 1.6
n_l^1	$0.170\,58 \pm 0.000\,11$	0.9556 ± 0.0014	2.9397 ± 0.0079	10.480 ± 0.064	25.92 ± 0.80
n_l^2	$0.056\,424$	$0.461\,23$	$3.035\,09$	18.7456	105.069
n_l^3	$0.006\,944\,4$	$0.075\,231$	$0.760\,54$	6.4263	53.496

Finally, we discuss the wave function renormalization for QED. It is obtained from the QCD result by adopting the following values for the QCD color factors:

$$C_F \to 1, \qquad C_A \to 0, \qquad T \to 1, \qquad d_F^{abcd} \to 1,$$
$$d_A^{abcd} \to 0, \qquad N_c \to 1. \tag{15}$$

We furthermore set $n_h = 1$ but keep the dependence on n_l. Note that $n_l = 0$ corresponds to the case of a massive electron and $n_l = 1$ describes the case of a massive muon and a massless electron. Our results are shown in Table II. For the n_l-independent part, we have an uncertainty of about 10%, and the n_l^1 term is determined with a 3% accuracy.

The on-shell wave function renormalization constant in QED has to be independent of ξ [5,27], which is fulfilled in our result as can be seen from the absence of all Abelian coefficients in Tables VI and VII; they are analytically zero. Note that the gauge parameter dependence only cancels after adding the mass counterterm contributions.

III. CHECKS AND HQET WAVE FUNCTION RENORMALIZATION

In this section, we describe several checks of our results. In particular, we discuss the relation to the wave function renormalization constant in HQET.

We start with the discussion of the $\overline{\rm MS}$ wave function renormalization constant $Z_2^{\overline{\rm MS}}$, which has been obtained to five-loop accuracy in Refs. [28,29]. In these papers, also the full ξ-dependence at four loops has been computed, which is crucial for our application. By definition, it only contains ultraviolet poles. On the other hand, as discussed in the Introduction, $Z_2^{\rm OS}$ contains both ultraviolet and infrared poles since it has to take care of both types of divergences in processes containing external heavy quarks. The ultraviolet divergences of $Z_2^{\rm OS}$ have to agree with the ones of $Z_2^{\overline{\rm MS}}$, and thus $Z_2^{\overline{\rm MS}}/Z_2^{\rm OS}$ only contains infrared poles. Note that the latter have to agree with the ultraviolet poles of the wave function renormalization constant in HQET, $Z_2^{\rm HQET}$, which can be seen as follows (see also the discussion in Ref. [5]): the off-shell heavy-quark propagator is infrared finite and contains only ultraviolet divergences, which can be renormalized in the $\overline{\rm MS}$ scheme; i.e., they are taken care of by $Z_2^{\overline{\rm MS}}$. If one applies an asymptotic expansion [30,31] around the on-shell limit, one obtains two contributions. The first one corresponds to a naive Taylor expansion of on-shell integrals which have to be evaluated in full QCD. It develops both ultraviolet and infrared divergences, as discussed above for the case of $Z_2^{\rm OS}$. The second contribution corresponds to HQET integrals and only has ultraviolet poles which have to cancel the infrared poles of the QCD contribution. Note that the wave functions $Z_2^{\rm OS}$ and $Z_2^{\rm HQET}$ considered in this paper correspond to the leading term in the expansion and thus $Z_2^{\rm HQET}/Z_2^{\rm OS}$ has to be infrared finite. As a consequence, the following combination of renormalization constants,

$$\frac{Z_2^{\overline{\rm MS}}}{Z_2^{\rm OS}} Z_2^{\rm HQET}, \tag{16}$$

has to be finite (see also the discussion in Ref. [32]). We will use this fact to determine the poles of $Z_2^{\rm HQET}$.

HQET describes the limit of QCD where the mass of the heavy quark goes to infinity. The heavy-quark field is integrated out from the Lagrange density. Thus, it is not a dynamical degree of freedom anymore. As a consequence, HQET contains as parameters the strong coupling constant and gauge parameter defined in the n_l-flavor theory, $\alpha_s^{(n_l)}$ and $\xi^{(n_l)}$.[1] Furthermore, there are no closed heavy-quark loops; i.e., color factors involving n_h are absent. Thus, when constructing (16), we can check that in the ratio $Z_2^{\overline{\rm MS}}/Z_2^{\rm OS}$ all color structures containing n_h are finite after using the decoupling relations for α_s and ξ [33]. At two- and three-loop order, this check can be performed analytically. At four loops, we observe that $Z_2^{\overline{\rm MS}}/Z_2^{\rm OS}$ is finite within our numerical precision. Note that this concerns the 11 color structures in Eq. (13) which are proportional to n_h, n_h^2, or n_h^3. Let us mention that all coefficients are zero within three standard deviations of the original FIESTA uncertainty, which means that in this case a security factor 3 would be sufficient.

The remaining 12 four-loop color structures are present in $Z_2^{\rm HQET}$, and the corresponding pole term can be extracted from Eq. (16). Before presenting the results, we remark that $Z_2^{\rm HQET}$ exponentiates according to [5,34]

$$\begin{aligned} Z_2^{\rm HQET} = \exp\Bigg\{ & x_1 C_F\left(\frac{\alpha_s}{\pi}\right) + C_F[x_2 C_A + x_3 T n_l]\left(\frac{\alpha_s}{\pi}\right)^2 + C_F[x_4 C_A^2 + x_5 C_A T n_l \\ & + x_6 T^2 n_l^2 + x_7 C_F T n_l]\left(\frac{\alpha_s}{\pi}\right)^3 + [C_F(x_8 C_A^3 + x_9 C_A^2 T n_l + x_{10} C_A T^2 n_l^2 \\ & + x_{11} T^3 n_l^3 + x_{12} C_F^2 T n_l + x_{13} C_F C_A T n_l + x_{14} C_F T^2 n_l^2) \\ & + x_{15} d_F^{abcd} d_A^{abcd}/N_c + x_{16} d_F^{abcd} d_F^{abcd} n_l/N_c]\left(\frac{\alpha_s}{\pi}\right)^4 + \cdots \Bigg\}, \end{aligned} \tag{17}$$

and thus there are only nine genuinely new color coefficients at four loops ($x_8, \ldots, x_{16}$) and the remaining three contributions proportional to C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$ can be predicted from lower loop orders. The comparison with the explicit calculation provides a strong check on our calculation. Note that the predictions of the C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$ contributions are available in analytic form.

In our practical calculations, we proceed as follows. In a first step, we use Eq. (16) to obtain a result for $Z_2^{\rm HQET}$ from the requirement that the combination of the three quantities is finite. Afterward, we use this result and compare to the expanded version of Eq. (17) to determine the coefficients x_i. Finally, we use Eq. (17) to predict the C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$ of $Z_2^{\rm HQET}$.

We refrain from providing explicit results for $Z_2^{\rm HQET}$ but provide our results for x_i in the ancillary file to this paper [25]. Furthermore, we present the expressions for the corresponding anomalous dimension, which is given by

$$\begin{aligned} \gamma_{\rm HQET} &= \frac{{\rm d}\log Z_2^{\rm HQET}}{{\rm d}\log \mu^2} \\ &= \sum_{n\ge 1} \gamma_{\rm HQET}^{(n)} \left(\frac{\alpha_s(\mu)}{\pi}\right)^n. \end{aligned} \tag{18}$$

Since our four-loop expression for $Z_2^{\rm HQET}$ is only known numerically, we have spurious ϵ poles in $\gamma_{\rm HQET}$. However, all of them are zero within two standard deviations of the uncertainty provided by FIESTA, which constitutes another useful cross-check for our calculation.

Let us in the following present our results for $\gamma_{\rm HQET}$. Up to three-loop order, we have

[1] Note that all quantities discussed in Sec. II depend on $n_f = n_l + n_h$ flavors.

TABLE III. Results for the different color factors of $\gamma^{(4)}_{\rm HQET}$. In columns 2 to 4, the coefficients of different powers of $\xi^{(n_l)}$ are given. In the uncertainties, a security factor 10 has been introduced.

	$(\xi^{(n_l)})^0$	$(\xi^{(n_l)})^1$	$(\xi^{(n_l)})^2$
$FAAA$	-2.03 ± 0.35	$-0.290\,37 \pm 0.000\,52$	$0.070\,83 \pm 0.000\,10$
d_{FA}	1.53 ± 0.84	0.5083 ± 0.0098	-0.1031 ± 0.0024
$d_{FF}L$	0.54 ± 0.26		
$FFFL$	0.1894 ± 0.0030		
$FFAL$	-0.4566 ± 0.0055	$-0.007\,663\,0$	
$FAAL$	2.576 ± 0.010	$0.251\,47$	$-0.010\,334\,8$
$FFLL$	$0.257\,25$		
$FALL$	$-0.537\,45$	$-0.007\,746\,0$	
$FLLL$	$-0.048\,262$		

$$\gamma^{(1)}_{\rm HQET} = -\frac{C_F}{2}\left(1+\frac{\xi^{(n_l)}}{2}\right),$$
$$\gamma^{(2)}_{\rm HQET} = C_F C_A\left(-\frac{19}{24}-\frac{5\xi^{(n_l)}}{32}+\frac{(\xi^{(n_l)})^2}{64}\right)+\frac{C_F T n_l}{3},$$
$$\gamma^{(3)}_{\rm HQET} = C_F C_A^2\left[-\frac{19\,495}{27\,648}-\frac{3\zeta_3}{16}-\frac{\pi^4}{360}+\xi^{(n_l)}\left(-\frac{379}{2048}-\frac{15\zeta_3}{256}+\frac{\pi^4}{1440}\right)+(\xi^{(n_l)})^2\left(\frac{69}{2048}+\frac{3\zeta_3}{512}\right)-\frac{5(\xi^{(n_l)})^3}{1024}\right]$$
$$+ C_F C_A T n_l\left(\frac{1105}{6912}+\frac{3\zeta_3}{4}+\frac{17\xi^{(n_l)}}{256}\right)+C_F^2 T n_l\left(\frac{51}{64}-\frac{3\zeta_3}{4}\right)+\frac{5C_F T^2 n_l^2}{108}, \qquad (19)$$

which agree with Refs. [5,34].

The four-loop terms to $\gamma_{\rm HQET}$ can be found in Table III, where for each color factor the coefficients of the $(\xi^{(n_l)})^k$ terms are shown together with their uncertainty. As for $Z_2^{\rm OS}$ in Sec. II, we have introduced a security factor 10. Note that the coefficients of $(\xi^{(n_l)})^k$ with $k \geq 3$ have not been computed.

We have the worst precision of about 50% for the color factors $d_F^{abcd} d_A^{abcd}$ and $n_l d_F^{abcd} d_F^{abcd}$ followed by $C_F C_A^3$, which is 17%. The relative uncertainty of the remaining n_l terms is much smaller. Note that the n_l^2 and n_l^3 terms are known analytically. They are obtained in a straightforward way for the corresponding analytic results for $Z_2^{\rm OS}$ from Ref. [17]. Our results read

$$\gamma^{(4),FFLL}_{\rm HQET} = \frac{3\zeta_3}{4}-\frac{\pi^4}{240}-\frac{103}{432},$$
$$\gamma^{(4),FALL}_{\rm HQET} = -\frac{35\zeta_3}{48}+\frac{\pi^4}{240}-\frac{4157}{62\,208}+\xi^{(n_l)}\left(-\frac{\zeta_3}{48}+\frac{269}{15\,552}\right),$$
$$\gamma^{(4),FLLL}_{\rm HQET} = \frac{1}{54}-\frac{\zeta_3}{18}. \qquad (20)$$

The expression for $\gamma^{(4),FFLL}_{\rm HQET}$ agrees with Refs. [35,36], and $\gamma^{(4),FLLL}_{\rm HQET}$ can be found in Ref. [37]. $\gamma^{(4),FALL}_{\rm HQET}$ is new.

Recently, also for the $n_l d_F^{abcd} d_F^{abcd}$ color structure, analytic results have been obtained [26]. The results read

$$\gamma^{(4),d_{FF}L}_{\rm HQET} = -\frac{5}{8}\zeta_5+\frac{1}{3}\pi^2\zeta_3+\frac{1}{2}\zeta_3-\frac{1}{3}\pi^2 \approx 0.617\,689\ldots \qquad (21)$$

and agrees well with our findings $\gamma^{(4),d_{FF}L}_{\rm HQET} \approx 0.54 \pm 0.26$. Note that here a security factor 2 would have been sufficient.

There are no contributions from the color structures C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$ to $\gamma^{(4)}_{\rm HQET}$ as is obvious by inspecting Eq. (17): the four-loop C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$ terms are generated by products of lower-order contributions. Since all coefficients x_i only contain poles in ϵ, the $1/\epsilon$ pole of $Z_2^{\rm HQET}$ does not involve C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$.

Let us finally compare the predicted C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$ contributions to $Z_2^{\rm HQET}$ to the ones we obtain by an explicit calculation. Table IV contains coefficients of $(\xi^{(n_l)})^k \epsilon^n$ for $k = 0$, 1, and 2 and for values of $n = -4$, $-3, \ldots$ up to one unit higher than the order up to which

TABLE IV. Contributions of the color structures C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$ to $Z_2^{\rm HQET}$. The coefficients of $(\xi^{(n_l)})^0$, $(\xi^{(n_l)})^1$, and $(\xi^{(n_l)})^2$ are given in rows 2 to 4. For each power of ϵ, the first row corresponds to the numerical evaluation of the analytic result, and the second row corresponds to the numerical result of our explicit calculation of $Z_2^{\rm OS}$. Relative uncertainties below 10^{-5} are set to zero. Note that the uncertainties in this paper are not multiplied by a security factor 10.

	$(\xi^{(n_l)})^0$	$(\xi^{(n_l)})^1$	$(\xi^{(n_l)})^2$
C_F^4			
$1/\epsilon^4$	0.002 604 2	0.005 208 3	0.003 906 3
	$0.002\,593\,2 \pm 0.000\,025$	0.005 208 3	0.003 906 3
$1/\epsilon^3$	0.000 00	0.000 00	0.000 00
	$0.000\,130\,49 \pm 0.000\,19$	0.000 00	0.000 00
$C_F^3 C_A$			
$1/\epsilon^4$	0.035 156	0.044 922	0.016 602
	$0.035\,190 \pm 0.000\,05$	0.044 922	0.016 602
$1/\epsilon^3$	−0.049 479	−0.059 245	−0.021 159
	$-0.049\,878 \pm 0.000\,44$	$-0.059\,245 \pm 0.000\,000\,06$	−0.021 159
$1/\epsilon^2$	0.000 00	0.000 00	0.000 00
	$0.002\,989\,3 \pm 0.0041$	$-0.000\,000\,2 \pm 0.000\,002\,0$	0.000 00
$C_F^2 C_A^2$			
$1/\epsilon^4$	0.130 914	0.085 558	0.002 726 2
	$0.130\,887 \pm 0.000\,04$	$0.085\,558 \pm 0.000\,000\,02$	0.002 726 2
$1/\epsilon^3$	−0.311 70	−0.191 497	−0.008 138 0
	$-0.311\,33 \pm 0.000\,35$	$-0.191\,497 \pm 0.000\,000\,2$	−0.008 138 0
$1/\epsilon^2$	0.278 52	0.162 322	0.008 824 1
	$0.276\,69 \pm 0.0033$	$0.162\,323 \pm 0.000\,002$	0.008 824 1
$1/\epsilon^1$	0.000 00	0.000 00	0.000 00
	0.046 ± 0.031	$-0.000\,014 \pm 0.000\,022$	0.000 00

the corresponding color structure has a nonzero contribution. The last ϵ order is shown as a check and demonstrates how well we can reproduce the 0. Note that in this table the displayed uncertainties are not multiplied by a security factor but correspond to the quadratically combined FIESTA uncertainties. In some cases, the relative uncertainty is very small and thus not shown at all. In all cases shown in Table IV, the numerical results agree within 1.5 sigma with the analytic predictions from Eq. (17). Note the color factors C_F^4, $C_F^3 C_A$, and $C_F^2 C_A^2$ get contributions from the most complicated master integrals, and thus the above comparison provides a strong check on the numerical setup of our calculation.

IV. CONCLUSIONS

We have computed four-loop QCD corrections to the wave function renormalization constant of heavy quarks, $Z_2^{\rm OS}$. Besides the on-shell quark mass renormalization constant and the leptonic anomalous magnetic moment, which have been considered in Refs. [1,2,7], respectively, this constitutes a third "classical" application of four-loop on-shell integrals. In the present calculation, we could have largely profited from the previous calculations. However, we had to deal with a more involved reduction to master integrals. Furthermore, we observed higher ϵ poles in the prefactors of some of the master integrals, which forced us to either change the basis or to expand the corresponding master integrals to higher order in ϵ.

$Z_2^{\rm OS}$ is neither gauge parameter independent nor infrared finite, which excludes two important checks used for $Z_m^{\rm OS}$ and the anomalous magnetic moment. However, a number of cross-checks are provided by the relation to the wave function renormalization constant of HQET.

In physical applications, $Z_2^{\rm OS}$ enters, among other quantities, as a building block. Most likely, in the evaluation of the other pieces, numerical methods play an important role as well, and thus various numerical pieces have to be combined to arrive at physical cross sections or decay rates. It might be that numerical cancellations take place, and thus, to date, it is not clear whether the numerical precision reached for $Z_2^{\rm OS}$ (which is of the order of 10^{-4} for $N_c = 3$) is sufficient for phenomenological applications. However, the results obtained in this paper serve for sure as important cross-checks for future more precise or even analytic calculations.

In the future, it would, of course, be desirable to obtain analytic results for fundamental quantities like on-shell QCD renormalization constants such as $Z_2^{\rm OS}$, which is considered in this paper, and $Z_m^{\rm OS}$ from Refs. [1,2]. First steps in this direction have been undertaken in Ref. [23] where a semianalytic approach has been used to obtain a high-precision result for the anomalous magnetic moment of the electron. One could imagine extending this analysis to the QCD-like master integrals.

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APPENDIX A: NUMERICAL RESULTS FOR Z_2^{OS}

Tables V, VI, VII, and VIII contain the numerical results for the coefficients of the individual color factors contributing to Z_2^{OS}.

TABLE V. Results for the coefficients of $\delta Z_2^{(4)}$ as defined in Eq. (13) for $\xi = 0$. A security factor 10 has been applied to the uncertainties.

	$1/\epsilon^4$	$1/\epsilon^3$	$1/\epsilon^2$	$1/\epsilon$	ϵ^0
$FFFF$	0.01317 ± 0.00025	0.0836 ± 0.0019	-0.084 ± 0.017	-1.96 ± 0.16	-4.1 ± 1.5
$FFFA$	-0.09665 ± 0.00053	-0.7611 ± 0.0044	-1.275 ± 0.041	1.10 ± 0.38	-9.8 ± 3.6
$FFAA$	0.21661 ± 0.00040	2.1150 ± 0.0035	9.698 ± 0.033	57.52 ± 0.31	324.5 ± 2.9
$FAAA$	-0.14442 ± 0.00011	-1.76642 ± 0.00096	-14.4491 ± 0.0092	-123.354 ± 0.086	-1007.40 ± 0.82
d_{FA}	-0.00002 ± 0.00029	0.0006 ± 0.0033	-0.002 ± 0.024	0.40 ± 0.21	9.4 ± 2.1
$d_{FF}L$	0.00001 ± 0.00011	-0.0001 ± 0.0014	0.0000 ± 0.0079	0.011 ± 0.064	-2.18 ± 0.80
$d_{FF}H$	-0.00001 ± 0.00023	0.0001 ± 0.0015	-0.001 ± 0.011	-0.120 ± 0.076	0.10 ± 0.50
$FFFL$	0.0351561 ± 0.0000013	0.2499987 ± 0.0000092	0.496651 ± 0.000077	0.39174 ± 0.00074	1.3920 ± 0.0067
$FFAL$	-0.1575519 ± 0.0000033	-1.457029 ± 0.000022	-7.60181 ± 0.00016	-46.0162 ± 0.0014	-236.417 ± 0.012
$FAAL$	0.1575515 ± 0.0000052	1.889980 ± 0.000070	17.10515 ± 0.00039	145.3220 ± 0.0026	1190.195 ± 0.031
$FFLL$	$0.028\,645\,8$	$0.244\,792$	$1.378\,40$	8.3824	40.329
$FALL$	-0.057292	-0.66059	-6.3943	-54.229	-447.65
$FLLL$	$0.006\,944\,4$	$0.075\,231$	$0.760\,54$	6.4263	53.496
$FFFH$	0.070313 ± 0.000023	0.255860 ± 0.000093	-0.65497 ± 0.00055	-3.8002 ± 0.0036	-5.953 ± 0.019
$FFAH$	-0.26173 ± 0.00010	-1.58102 ± 0.00044	-3.2136 ± 0.0021	-11.729 ± 0.013	-26.860 ± 0.083
$FAAH$	0.215336 ± 0.000061	1.95402 ± 0.00027	11.5396 ± 0.0014	70.3186 ± 0.0091	424.301 ± 0.056
$FFHH$	0.0937498 ± 0.0000014	0.2109378 ± 0.0000059	-0.329095 ± 0.000035	-0.57438 ± 0.00013	-7.99681 ± 0.00079
$FAHH$	-0.117186 ± 0.000011	-0.681863 ± 0.000054	-2.52735 ± 0.00029	-10.3208 ± 0.0012	-40.2646 ± 0.0062
$FHHH$	$0.027\,777\,8$	$0.047\,454$	$0.173\,582$	$0.276\,902$	$0.612\,12$
$FFLH$	$0.093\,750$	$0.507\,81$	1.3923245 ± 0.0000012	5.834231 ± 0.000010	8.990228 ± 0.000074
$FALH$	-0.1545138 ± 0.0000011	-1.3179979 ± 0.0000063	-9.088033 ± 0.000034	-56.32679 ± 0.00020	-344.7315 ± 0.0015
$FLLH$	$0.027\,777\,8$	$0.216\,435$	$1.656\,69$	10.3632	64.740
$FLHH$	$0.041\,667$	$0.197\,917$	$1.050\,74$	4.2433	17.7160

TABLE VI. Same as in Table V but the coefficients of the linear ξ terms.

	$1/\epsilon^4$	$1/\epsilon^3$	$1/\epsilon^2$	$1/\epsilon$	ϵ^0
$FFFA$	0	0	-0.000000 ± 0.000020	0.00001 ± 0.00020	-0.0001 ± 0.0011
$FFAA$	0	-0.0000001 ± 0.0000016	-0.005369 ± 0.000022	-0.03679 ± 0.00022	-0.3166 ± 0.0012
$FAAA$	0	-0.0000001 ± 0.0000039	0.013200 ± 0.000023	0.11976 ± 0.00013	1.42164 ± 0.00076
d_{FA}	-0.0000003 ± 0.0000100	0.000005 ± 0.000088	-0.00000 ± 0.00051	0.1135 ± 0.0025	0.147 ± 0.013
$FAAL$	0	0	-0.0035799	-0.033281	-0.40121
$FFAH$	$0.003\,906\,2$	-0.0094401	0.0069760 ± 0.0000032	0.037345 ± 0.000035	-0.76089 ± 0.00024
$FAAH$	-0.0052626	$0.011\,203\,4$	-0.0854353 ± 0.0000018	0.216644 ± 0.000018	-1.40360 ± 0.00013
$FAHH$	$0.002\,604\,17$	-0.0078125	$0.047\,919$	-0.182917	$0.789\,80$
$FALH$	$0.001\,7361\,1$	-0.0052083	$0.043\,906$	-0.148948	$0.796\,19$

TABLE VII. Same as in Table V but the coefficients of ξ^2.

	$1/\epsilon^4$	$1/\epsilon^3$	$1/\epsilon^2$	$1/\epsilon$	ϵ^0
$FAAA$	0	0.0000000 ± 0.0000011	-0.0006711 ± 0.0000052	-0.005817 ± 0.000025	-0.07062 ± 0.00012
d_{FA}	0.0000002 ± 0.0000038	-0.000001 ± 0.000026	-0.00000 ± 0.00012	-0.01250 ± 0.00061	-0.0748 ± 0.0028
$FAAH$	0	$0.000\,325\,52$	-0.00100945	$0.008\,971\,5$	-0.032896

TABLE VIII. Results for the coefficients of $\delta Z_2^{(4)}$ as defined in Eq. (13) for $\xi = 0$ and without taking into account the mass counterterms from lower loop orders. A security factor 10 has been applied to the uncertainties.

	$1/\epsilon^4$	$1/\epsilon^3$	$1/\epsilon^2$	$1/\epsilon$	ϵ^0
$FFFF$	−2.731 94 ± 0.000 25	1.9450 ± 0.0019	−22.265 ± 0.017	93.41 ± 0.16	167.9 ± 1.5
$FFFA$	−2.627 90 ± 0.000 53	−4.6110 ± 0.0044	−48.022 ± 0.041	−74.51 ± 0.38	−618.5 ± 3.6
$FFAA$	−1.029 81 ± 0.000 40	−5.9684 ± 0.0035	−44.525 ± 0.033	−255.18 ± 0.31	−1664.9 ± 2.9
$FAAA$	−0.144 42 ± 0.000 11	−1.766 42 ± 0.000 96	−14.4491 ± 0.0092	−123.354 ± 0.086	−1007.40 ± 0.82
d_{FA}	−0.000 02 ± 0.000 29	0.0006 ± 0.0033	−0.002 ± 0.024	0.40 ± 0.21	9.4 ± 2.1
$d_{FF}L$	0.000 01 ± 0.000 11	−0.0001 ± 0.0014	0.0000 ± 0.0079	0.011 ± 0.064	−2.18 ± 0.80
$d_{FF}H$	−0.000 01 ± 0.000 23	0.0001 ± 0.0015	−0.001 ± 0.011	−0.120 ± 0.076	0.10 ± 0.50
$FFFL$	1.312 499 9 ± 0.000 001 3	2.650 389 3 ± 0.000 009 2	31.883 671 ± 0.000 077	55.083 00 ± 0.000 74	477.6787 ± 0.0067
$FFAL$	0.875 000 2 ± 0.000 003 3	4.729 724 ± 0.000 022	42.827 31 ± 0.000 16	217.1492 ± 0.0014	1568.153 ± 0.012
$FAAL$	0.157 551 5 ± 0.000 005 2	1.889 980 ± 0.000 070	17.105 15 ± 0.000 39	145.3220 ± 0.0026	1190.195 ± 0.031
$FFLL$	−0.179 688	−0.882 81	−9.3076	−43.714	−340.67
$FALL$	−0.057 292	−0.660 59	−6.3943	−54.229	−447.65
$FLLL$	0.006 944 4	0.075 231	0.760 54	6.4263	53.496
$FFFH$	2.156 250 ± 0.000 023	1.492 579 ± 0.000 093	20.691 69 ± 0.000 55	9.3957 ± 0.0036	92.254 ± 0.019
$FFAH$	1.229 16 ± 0.000 10	4.778 52 ± 0.000 44	26.4927 ± 0.0021	101.634 ± 0.013	487.440 ± 0.083
$FAAH$	0.2153 36 ± 0.000 061	1.954 02 ± 0.000 27	11.5396 ± 0.0014	70.3186 ± 0.0091	424.301 ± 0.056
$FFHH$	−0.416 666 9 ± 0.000 001 4	−0.648 437 2 ± 0.000 005 9	−3.496 296 ± 0.000 035	−7.428 24 ± 0.000 13	−20.152 61 ± 0.000 79
$FAHH$	−0.117 186 ± 0.000 011	−0.681 863 ± 0.000 054	−2.527 35 ± 0.000 29	−10.3208 ± 0.0012	−40.2646 ± 0.0062
$FHHH$	0.027 777 8	0.047 454	0.173 582	0.276 902	0.612 12
$FFLH$	−0.505 21	−1.687 50	−13.148 579 4 ± 0.000 001 2	−44.062 536 ± 0.000 010	−243.607 004 ± 0.000 074
$FALH$	−0.154 513 8 ± 0.000 001 1	−1.317 997 9 ± 0.000 006 3	−9.088 033 ± 0.000 034	−56.326 79 ± 0.000 20	−344.7315 ± 0.0015
$FLLH$	0.027 777 8	0.216 435	1.656 69	10.3632	64.740
$FLHH$	0.041 667	0.197 917	1.050 74	4.2433	17.7160

APPENDIX B: $Z_2^{\rm OS}$ TO THREE LOOPS

In this Appendix, we provide results for the coefficients of $Z_2^{\rm OS}$ as defined in Eq. (9) up to three loops including higher-order terms in ϵ; the n-loop expression contains terms up to order ϵ^{4-n}. Note that in Eq. (9) the quark mass M is renormalized on shell but α_s is bare. Our results read

$$\delta Z_2^{(1)} = \left(\frac{\zeta_3}{3}-\frac{3\pi^4}{640}-\frac{\pi^2}{6}-8\right)\epsilon^3 C_F + \left(\frac{\zeta_3}{4}-\frac{\pi^2}{12}-4\right)\epsilon^2 C_F + \left(-2-\frac{\pi^2}{16}\right)\epsilon C_F - \frac{3C_F}{4\epsilon} - C_F, \tag{B1}$$

$$\begin{aligned}
\delta Z_2^{(2)} = {}& \epsilon\Bigg(C_A C_F\left(12a_4+\frac{199\zeta_3}{24}-\frac{7\pi^4}{40}+\frac{227\pi^2}{384}-\frac{4241}{256}+\frac{\log^4(2)}{2}+\pi^2\log^2(2)-\frac{23}{8}\pi^2\log(2)\right)\\
&+C_F^2\left(-24a_4-\frac{297\zeta_3}{16}+\frac{7\pi^4}{20}-\frac{339\pi^2}{128}+\frac{211}{256}-\log^4(2)-2\pi^2\log^2(2)+\frac{23}{4}\pi^2\log(2)\right)\\
&+C_F\left(-\frac{43\zeta_3}{6}-\frac{437\pi^2}{288}+\frac{20\,275}{1728}+2\pi^2\log(2)\right)T_F n_h+\left(\frac{11\zeta_3}{12}+\frac{15\pi^2}{32}+\frac{369}{64}\right)C_F T_F n_l\Bigg)\\
&+\epsilon^2\Bigg(C_A C_F\Bigg(69a_4+72a_5-\frac{11\pi^2\zeta_3}{8}+\frac{2561\zeta_3}{96}-\frac{609\zeta_5}{8}-\frac{7229\pi^4}{11520}\\
&+\frac{2005\pi^2}{768}-\frac{30163}{512}-\frac{3\log^5(2)}{5}+\frac{23\log^4(2)}{8}-2\pi^2\log^3(2)+\frac{23}{4}\pi^2\log^2(2)+\frac{13}{30}\pi^4\log(2)-\frac{41}{4}\pi^2\log(2)\Bigg)\\
&+C_F^2\Bigg(-138a_4-144a_5+\frac{11\pi^2\zeta_3}{4}-\frac{2069\zeta_3}{32}+\frac{609\zeta_5}{4}+\frac{3901\pi^4}{3840}\\
&-\frac{8851\pi^2}{768}+\frac{4889}{512}+\frac{6\log^5(2)}{5}-\frac{23\log^4(2)}{4}+4\pi^2\log^3(2)-\frac{23}{2}\pi^2\log^2(2)-\frac{13}{15}\pi^4\log(2)+\frac{41}{2}\pi^2\log(2)\Bigg)\\
&+C_F T_F n_h\left(-48a_4-\frac{2413\zeta_3}{72}+\frac{47\pi^4}{160}-\frac{8509\pi^2}{1728}+\frac{450\,395}{10\,368}-2\log^4(2)-4\pi^2\log^2(2)+\frac{19}{2}\pi^2\log(2)\right)\\
&+\left(\frac{33\zeta_3}{8}+\frac{101\pi^4}{960}+\frac{295\pi^2}{192}+\frac{2259}{128}\right)C_F T_F n_l\Bigg)\\
&+C_A C_F\left(\frac{3\zeta_3}{4}+\frac{49\pi^2}{192}-\frac{803}{128}-\frac{1}{2}\pi^2\log(2)\right)\\
&+C_F^2\left(-\frac{3\zeta_3}{2}-\frac{49\pi^2}{64}+\frac{433}{128}+\pi^2\log(2)\right)+\left(\frac{1139}{288}-\frac{7\pi^2}{24}\right)C_F T_F n_h\\
&+\left(\frac{59}{32}+\frac{5\pi^2}{48}\right)C_F T_F n_l\\
&+\frac{-\frac{11C_AC_F}{32}+\frac{1}{4}C_F T_F n_h+\frac{1}{8}C_F T_F n_l+\frac{9C_F^2}{32}}{\epsilon^2}\\
&+\frac{-\frac{101C_AC_F}{64}+\frac{19}{48}C_F T_F n_h+\frac{9}{16}C_F T_F n_l+\frac{51C_F^2}{64}}{\epsilon},
\end{aligned}\tag{B2}$$

$$\begin{aligned}
\delta Z_2^{(3)} = {}& \left(-10a_4+\frac{\pi^2\zeta_3}{8}-\frac{739\zeta_3}{128}-\frac{5\zeta_5}{16}-\frac{5\log^4(2)}{12}+3\pi^2\log^2(2)+\frac{685}{48}\pi^2\log(2)-\frac{41\pi^4}{120}-\frac{58\,321\pi^2}{9216}-\frac{10\,823}{3072}\right)C_F^3\\
&+C_A\Bigg(-\frac{319a_4}{6}-\frac{45\pi^2\zeta_3}{16}-\frac{19\,981\zeta_3}{384}+\frac{145\zeta_5}{16}-\frac{319\log^4(2)}{144}-\frac{499}{72}\pi^2\log^2(2)\\
&+\frac{2281}{288}\pi^2\log(2)+\frac{20\,053\pi^4}{17\,280}-\frac{15\,053\pi^2}{9216}+\frac{150\,871}{9216}\Bigg)C_F^2
\end{aligned}$$

$$+ T_F n_l \left(\frac{64 a_4}{3} + \frac{1661 \zeta_3}{96} + \frac{8 \log^4(2)}{9} + \frac{16}{9}\pi^2 \log^2(2) - \frac{58}{9}\pi^2 \log(2) - \frac{733\pi^4}{2160} + \frac{6931\pi^2}{2304} - \frac{3773}{2304} \right) C_F^2$$

$$+ T_F n_h \left(28 a_4 + \frac{5327\zeta_3}{288} + \frac{7\log^4(2)}{6} + \frac{5}{6}\pi^2\log^2(2) - \frac{31}{9}\pi^2 \log(2) - \frac{137\pi^4}{720} + \frac{25\,223\pi^2}{20\,736} - \frac{78\,967}{6912} \right) C_F^2$$

$$+ T_F^2 n_l^2 \left(-\frac{37\zeta_3}{36} - \frac{23\pi^2}{48} - \frac{4025}{972} \right) C_F + T_F^2 n_h n_l \left(\frac{49\zeta_3}{12} - \frac{4}{3}\pi^2 \log(2) + \frac{77\pi^2}{72} - \frac{1168}{81} \right) C_F$$

$$+ T_F^2 n_h^2 \left(\frac{85\zeta_3}{12} - \frac{4}{3}\pi^2 \log(2) + \frac{767\pi^2}{720} - \frac{6887}{648} \right) C_F + C_A T_F n_h \left(-16 a_4 + \xi \left(-\frac{7\zeta_3}{192} + \frac{\pi^2}{256} + \frac{407}{1728} \right) \right.$$

$$\left. + \frac{11\pi^2\zeta_3}{48} - \frac{3359\zeta_3}{144} - \frac{15\zeta_5}{16} - \frac{2\log^4(2)}{3} - \frac{1}{3}\pi^2\log^2(2) + \frac{521}{36}\pi^2 \log(2) + \frac{5\pi^4}{72} - \frac{105\,359\pi^2}{10\,368} + \frac{32\,257}{648} \right) C_F$$

$$+ C_A T_F n_l \left(-\frac{32 a_4}{3} - \frac{301\zeta_3}{72} - \frac{4\log^4(2)}{9} - \frac{8}{9}\pi^2\log^2(2) + \frac{29}{9}\pi^2 \log(2) + \frac{29\pi^4}{216} + \frac{2413\pi^2}{3456} + \frac{416\,405}{15\,552} \right) C_F$$

$$+ C_A^2 \left(\frac{349 a_4}{12} + \frac{127\pi^2\zeta_3}{72} + \frac{3623\zeta_3}{144} + \xi \left(\frac{\pi^2\zeta_3}{144} - \frac{13\zeta_3}{256} + \frac{7\zeta_5}{384} + \frac{17\pi^4}{27\,648} - \frac{\pi^2}{256} - \frac{13}{768} \right) \right.$$

$$\left. - \frac{37\zeta_5}{6} + \frac{349\log^4(2)}{288} + \frac{391}{144}\pi^2\log^2(2) - \frac{271}{36}\pi^2 \log(2) - \frac{10\,811\pi^4}{23\,040} - \frac{107\pi^2}{864} - \frac{2\,551\,697}{62\,208} \right) C_F$$

$$+ \frac{1}{\epsilon^3} \left[-\frac{9 C_F^3}{128} + \frac{33}{128} C_A C_F^2 - \frac{3}{16} T_F n_h C_F^2 - \frac{3}{32} T_F n_l C_F^2 - \frac{121}{576} C_A^2 C_F \right.$$

$$\left. - \frac{1}{12} T_F^2 n_h^2 C_F - \frac{1}{36} T_F^2 n_l^2 C_F + \frac{11}{72} C_A T_F n_l C_F - \frac{1}{12} T_F^2 n_h n_l C_F + C_A T_F n_h \left(\frac{15}{64} - \frac{\xi}{192} \right) C_F \right]$$

$$+ \frac{1}{\epsilon^2} \left[-\frac{81 C_F^3}{256} + \frac{1217}{768} C_A C_F^2 - \frac{91}{192} T_F n_h C_F^2 - \frac{103}{192} T_F n_l C_F^2 - \frac{1501}{864} C_A^2 C_F \right.$$

$$\left. - \frac{5}{36} T_F^2 n_h^2 C_F - \frac{23}{108} T_F^2 n_l^2 C_F + \frac{1069}{864} C_A T_F n_l C_F - \frac{7}{18} T_F^2 n_h n_l C_F + C_A T_F n_h \left(\frac{\xi}{64} + \frac{353}{288} \right) C_F \right]$$

$$+ \frac{1}{\epsilon} \left[\left(\frac{9\zeta_3}{8} - \frac{3}{4}\pi^2 \log(2) + \frac{303\pi^2}{512} - \frac{1039}{512} \right) C_F^3 + T_F n_l \left(\frac{3\zeta_3}{4} - \frac{2}{3}\pi^2 \log(2) + \frac{175\pi^2}{384} - \frac{351}{128} \right) C_F^2 \right.$$

$$+ T_F n_h \left(\zeta_3 - \frac{2}{3}\pi^2 \log(2) + \frac{143\pi^2}{192} - \frac{1525}{384} \right) C_F^2 + C_A \left(-\frac{27\zeta_3}{8} + \frac{53}{24}\pi^2 \log(2) - \frac{2549\pi^2}{1536} + \frac{14\,887}{1536} \right) C_F^2$$

$$+ C_A^2 \left(\xi \left(-\frac{3\zeta_3}{256} + \frac{\pi^4}{4320} - \frac{1}{768} \right) + \frac{173\zeta_3}{128} - \frac{11}{12}\pi^2 \log(2) - \frac{\pi^4}{1080} + \frac{1199\pi^2}{2304} - \frac{55\,945}{5184} \right) C_F$$

$$+ C_A T_F n_h \left(\left(-\frac{35}{576} - \frac{\pi^2}{768} \right) \xi - \frac{\zeta_3}{2} + \frac{1}{3}\pi^2 \log(2) - \frac{1753\pi^2}{2304} + \frac{503}{48} \right) C_F$$

$$+ C_A T_F n_l \left(-\frac{\zeta_3}{4} + \frac{1}{3}\pi^2 \log(2) - \frac{5\pi^2}{288} + \frac{550}{81} \right) C_F + T_F^2 n_h^2 \left(-\frac{131}{54} + \frac{29\pi^2}{144} \right) C_F$$

$$\left. + T_F^2 n_h n_l \left(-\frac{31}{9} + \frac{7\pi^2}{48} \right) C_F + T_F^2 n_l^2 \left(-\frac{325}{324} - \frac{\pi^2}{16} \right) C_F \right]$$

$$+ \epsilon \left(\left(\frac{29\zeta_3^2}{32} + 14\pi^2 \log(2)\zeta_3 + \frac{5267\pi^2\zeta_3}{288} - \frac{69\,511\zeta_3}{256} - \frac{4267 a_4}{6} - \frac{116 a_5}{3} \right. \right.$$

$$- \frac{1403\zeta_5}{16} + \frac{29\log^5(2)}{90} + \frac{2}{3}\pi^2\log^4(2) - \frac{4267\log^4(2)}{144} - \frac{196}{27}\pi^2\log^3(2)$$

$$- \frac{2}{3}\pi^4\log^2(2) - \frac{3997}{72}\pi^2\log^2(2) - \frac{2351\pi^4 \log(2)}{2160} + \frac{1345}{8}\pi^2 \log(2) - \frac{899\pi^6}{5670}$$

$$
\begin{aligned}
&+\frac{450\,893\pi^4}{552\,960}+16a_4\pi^2-\frac{56\,455\pi^2}{2048}-\frac{108\,677}{6144}\bigg)C_F^3\\
&+T_Fn_l\bigg(\frac{1856a_4}{9}+\frac{512a_5}{3}-\frac{69\pi^2\zeta_3}{16}+\frac{57\,581\zeta_3}{576}-\frac{2245\zeta_5}{12}-\frac{64\log^5(2)}{45}\\
&+\frac{232\log^4(2)}{27}-\frac{128}{27}\pi^2\log^3(2)+\frac{464}{27}\pi^2\log^2(2)+\frac{139}{270}\pi^4\log(2)-\frac{908}{27}\pi^2\log(2)\\
&-\frac{610\,451\pi^4}{414\,720}+\frac{251\,107\pi^2}{13\,824}-\frac{36\,677}{13\,824}\bigg)C_F^2\\
&+T_Fn_h\bigg(\frac{539a_4}{6}+168a_5-\frac{287\pi^2\zeta_3}{24}+\frac{1087\zeta_3}{96}-\frac{899\zeta_5}{8}-\frac{7\log^5(2)}{5}\\
&+\frac{539\log^4(2)}{144}-\frac{5}{3}\pi^2\log^3(2)-\frac{683}{144}\pi^2\log^2(2)+\frac{247}{180}\pi^4\log(2)+\frac{673}{24}\pi^2\log(2)\\
&-\frac{32\,857\pi^4}{69\,120}-\frac{341\,735\pi^2}{41\,472}-\frac{143\,029}{13\,824}\bigg)C_F^2\\
&+C_A\bigg(-\frac{143\zeta_3^2}{4}+\frac{21}{4}\pi^2\log(2)\zeta_3-\frac{5777\pi^2\zeta_3}{384}-\frac{188\,083\zeta_3}{2304}-\frac{3787a_4}{36}\\
&-\frac{1441a_5}{3}+\frac{254\,581\zeta_5}{384}+\frac{1441\log^5(2)}{360}+\frac{1}{4}\pi^2\log^4(2)-\frac{3787\log^4(2)}{864}\\
&+\frac{2089}{108}\pi^2\log^3(2)-\frac{1}{4}\pi^4\log^2(2)-\frac{25\,441}{432}\pi^2\log^2(2)-\frac{559}{540}\pi^4\log(2)\\
&-\frac{5623}{216}\pi^2\log(2)-\frac{27\,331\pi^6}{181\,440}+\frac{11\,810\,161\pi^4}{1\,658\,880}+6a_4\pi^2-\frac{1\,265\,393\pi^2}{55\,296}+\frac{4\,824\,655}{55\,296}\bigg)C_F^2\\
&+T_F^2n_l^2\bigg(-\frac{851\zeta_3}{108}-\frac{535\pi^4}{3456}-\frac{325\pi^2}{144}-\frac{23\,789}{1458}\bigg)C_F\\
&+T_F^2n_hn_l\bigg(\frac{128a_4}{3}+\frac{595\zeta_3}{18}+\frac{16\log^4(2)}{9}+\frac{32}{9}\pi^2\log^2(2)-\frac{92}{9}\pi^2\log(2)-\frac{341\pi^4}{3456}+\frac{145\pi^2}{36}-\frac{17\,740}{243}\bigg)C_F\\
&+T_F^2n_h^2\bigg(\frac{152a_4}{3}+\frac{25\,723\zeta_3}{720}+\frac{19\log^4(2)}{9}+\frac{17}{9}\pi^2\log^2(2)-\frac{33}{5}\pi^2\log(2)-\frac{391\pi^4}{1152}+\frac{83\,227\pi^2}{16\,200}-\frac{1\,023\,397}{19\,440}\bigg)C_F\\
&+C_A^2\bigg(\frac{7451\zeta_3^2}{384}-\frac{49}{8}\pi^2\log(2)\zeta_3+\frac{3299\pi^2\zeta_3}{4608}+\frac{236\,171\zeta_3}{3456}+\frac{4147a_4}{18}+\frac{1499a_5}{6}\\
&+\xi\bigg(\frac{25\zeta_3^2}{384}+\frac{77\pi^2\zeta_3}{9216}-\frac{63\zeta_3}{256}-\frac{149\zeta_5}{768}+\frac{49\pi^6}{51\,840}+\frac{383\pi^4}{138\,240}-\frac{35\pi^2}{1024}-\frac{35}{256}\bigg)\\
&-\frac{77\,297\zeta_5}{256}-\frac{1499\log^5(2)}{720}-\frac{7}{24}\pi^2\log^4(2)+\frac{4147\log^4(2)}{432}-\frac{1697}{216}\pi^2\log^3(2)\\
&+\frac{7}{24}\pi^4\log^2(2)+\frac{4679}{108}\pi^2\log^2(2)+\frac{6823\pi^4\log(2)}{8640}-\frac{25\,069}{864}\pi^2\log(2)\\
&+\frac{45\,047\pi^6}{362\,880}-\frac{2\,973\,217\pi^4}{829\,440}-7a_4\pi^2+\frac{26\,425\pi^2}{20\,736}-\frac{74\,570\,603}{373\,248}\bigg)C_F\\
&+C_AT_Fn_l\bigg(-\frac{928a_4}{9}-\frac{256a_5}{3}+\frac{77\pi^2\zeta_3}{48}-\frac{11\,159\zeta_3}{864}+\frac{2077\zeta_5}{24}+\frac{32\log^5(2)}{45}-\frac{116\log^4(2)}{27}+\frac{64}{27}\pi^2\log^3(2)\\
&-\frac{232}{27}\pi^2\log^2(2)-\frac{139}{540}\pi^4\log(2)+\frac{454}{27}\pi^2\log(2)+\frac{122\,131\pi^4}{103\,680}+\frac{10\,535\pi^2}{2592}+\frac{10\,805\,903}{93\,312}\bigg)C_F
\end{aligned}
$$

$$
\begin{aligned}
&+C_A T_F n_h\left(\frac{181\zeta_3^2}{32}+7\pi^2\log(2)\zeta_3+\frac{1823\pi^2\zeta_3}{192}-\frac{357\,881\zeta_3}{1152}-\frac{5855a_4}{12}-96a_5\right.\\
&+\xi\left(\frac{7\zeta_3}{64}+\frac{173\pi^4}{92\,160}-\frac{35\pi^2}{2304}-\frac{4859}{5184}\right)+\frac{2697\zeta_5}{64}+\frac{4\log^5(2)}{5}+\frac{1}{3}\pi^2\log^4(2)\\
&-\frac{5855\log^4(2)}{288}+\frac{2}{3}\pi^2\log^3(2)-\frac{1}{3}\pi^4\log^2(2)-\frac{21\,349}{288}\pi^2\log^2(2)-\frac{149}{180}\pi^4\log(2)\\
&\left.+\frac{3973}{36}\pi^2\log(2)-\frac{1501\pi^6}{15120}+\frac{173\,713\pi^4}{55\,296}+8a_4\pi^2-\frac{163\,981\pi^2}{5184}+\frac{1\,004\,165}{3888}\right)C_F\Bigg), \qquad \text{(B3)}
\end{aligned}
$$

where $C_F=(N_c^2-1)/(2N_c)$ and $C_A=N_c$ are the eigenvalues of the quadratic Casimir operators of the fundamental and adjoint representation for the $SU(N_c)$ color group, respectively; $T=1/2$ is the index of the fundamental representation; and n_l and n_h count the number of massless and massive (with mass M) quarks. It is convenient to keep the variable n_h as a parameter, although in our case, we have $n_h=1$. Computer-readable expressions of $\delta Z_2^{(1)}$, $\delta Z_2^{(2)}$, and $\delta Z_2^{(3)}$ can be found in Ref. [25].

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