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Renormalization of twist-two operators and four-loop splitting functions in QCD

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The scale evolution of parton distribution functions is governed by the splitting functions. One of the most efficient methods is to extract splitting functions via the computations of off-shell operator matrix elements, where the physical twist-two operators mix with some unknown gauge-variant operators. We proposed a new method to systematically extract the counterterm Feynman rules resulting from those gauge-variant operators. As a first application of the new method, we rederived the three-loop singlet unpolarized splitting functions. As another application, we obtained a new result for the four-loop pure-singlet splitting functions with two closed fermionic loops. We also presented a new result for the $N_f C_F^3$ contribution to the four-loop non-singlet splitting function, where the gauge-variant operators are absent.

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1. Background

The theory predictions of all high-energy hadronic collider observables rely on the factorization theorem in Quantum Chromodynamics (QCD), which expresses the hadronic cross section as the convolutions of the universal parton distribution functions (PDFs) and partonic cross sections. The partonic cross sections can be calculated from the first principle in perturbative QCD. The PDFs are non-perturbative quantities and they are hard to determine. Still, their scale evolution (the well-known DGLAP evolution [1–3]) is governed by splitting functions, which can be evaluated perturbatively in QCD.

The calculations of partonic cross sections have received rapid progress. Several benchmark partonic cross sections in QCD have been evaluated to next-to-next-to-next-to-leading order ($\mathrm{N^3LO}$). To obtain the same precision for hadronic cross sections, it is necessary to know the $\mathrm{N^3LO}$ PDFs, which require the knowledge of four-loop splitting functions. The splitting functions at three-loop accuracy in QCD were computed almost 20 years ago [4, 5], and allowed the complete determination of NNLO PDFs. At four-loop order, only partial results are available [6–17]. Those results were already used to obtain approximate $\mathrm{N^3LO}$ PDFs [18, 19].

Traditionally, the splitting functions were extracted from physical partonic cross-sections. This method is technically complicated and challenges the current computational power, memory, and storage demands, see for example, [15]. It is thus desirable to search for more efficient methods to determine the four-loop splitting functions. One of the most efficient methods is to extract splitting functions via the computations of off-shell operator matrix elements (OMEs), in the framework of operator product expansion (OPE). The off-shell OMEs are defined as the off-shell OMEs with a single operator insertion, for the case of two partons in the external states it is

$$A_{ij} = \langle j(p)|O_i|j(p)\rangle \ \text{ with } p^2 < 0\,, \tag{1}$$

where O_i is a twist-two operator. The twist-two operators are classified into non-singlet and singlet operators according to flavor group $SU(N_f)$. There is one non-singlet spin-n quark operator

$$O_{\rm ns}(n) = \frac{i^{n-1}}{2}\left[\bar{\psi}_{i_1}\Delta\cdot\gamma(\Delta\cdot D)_{i_1 i_2}(\Delta\cdot D)_{i_2 i_3}\cdots(\Delta\cdot D)_{i_{n-1}i_n}\frac{\lambda_k}{2}\psi_{i_n}\right],\ k = 3,\cdots N_f^2-1\,, \tag{2}$$

and two singlet quark and gluon operators

$$\begin{aligned} O_q(n) &= \frac{i^{n-1}}{2}\left[\bar{\psi}_{i_1}\Delta\cdot\gamma(\Delta\cdot D^{\mu})_{i_1 i_2}(\Delta\cdot D)_{i_2 i_3}\cdots(\Delta\cdot D)_{i_{n-1}i_n}\psi_{i_n}\right],\\ O_g(n) &= -\frac{i^{n-2}}{2}\left[\Delta_{\mu_1}\cdot G^{\mu_1}_{a_1,\mu}(\Delta\cdot D)_{a_1 a_2}\cdots(\Delta\cdot D)_{a_{n-2}a_{n-1}}\Delta_{\mu_n}G^{\mu_n\mu}_{a_{n-1}a_n}\right]. \end{aligned} \tag{3}$$

In the above equations, $\lambda_k/2$ denotes diagonal generators of the flavor group $\mathrm{SU}(N_f)$, and Δ is a light-like reference vector with $\Delta^2 = 0$. The symbol ψ and G represent the quark field and gluon field strength tensor respectively, and $D^\mu = \partial_\mu\,\delta - i g_s \boldsymbol{T}^a A^a_\mu$ is the covariant derivative in the fundamental or adjoint representations of a general gauge group.

The non-singlet sector allows for a direct multiplicative renormalization:

$$O^{\rm R}_{\rm ns}(\mu, n) = Z_{\rm ns}(\mu, n) O^{\rm B}_{\rm ns}(n)\,, \tag{4}$$

where superscripts B and R are used to represent the bare and renormalized operators, respectively. Naively, one would expect that the renormalization in the singlet sector reads

$$\begin{pmatrix} O_q \\ O_g \end{pmatrix}^{\text{R,naive}} = \begin{pmatrix} Z_{qq} & Z_{qg} \\ Z_{gq} & Z_{gg} \end{pmatrix} \begin{pmatrix} O_q \\ O_g \end{pmatrix}^{\text{B}} . \tag{5}$$

In the following, we will see the above renormalization procedure needs to be extended if we work with the off-shell external states.

The renormalized operators satisfy a renormalization group equation,

$$\frac{dO^{\text{R}}(\mu,n)}{d\ln\mu} = -2\gamma(\mu,n)\cdot O^{\text{R}}(\mu,n)\,, \tag{6}$$

which defines the anomalous dimensions $\gamma(n)$ of the twist-two operators. The anomalous dimensions $\gamma(n)$ with Mellin moments n are related to splitting functions $P(x)$ via the following Mellin transformation,

$$\gamma(\mu,n) = -\int_0^1 dx x^{n-1} P(\mu,x)\,. \tag{7}$$

The anomalous dimension $\gamma = \gamma_{\text{ns}}$ is a scalar in the non-singlet case, and is a two-by-two matrix with elements γ_{ij} $(i,\ j = q,\ g)$ in the singlet sector. Since the bare operators don't depend on the renormalization scale μ, it is easy to show that the associated renormalization constants satisfy the following renormalization group equation:

$$\frac{dZ(\mu,n)}{d\ln\mu} = -2\gamma(\mu,n)\cdot Z(\mu,n)\,. \tag{8}$$

With the help of the d-dimensional QCD β function

$$\beta(a_s,\,\epsilon) = \frac{da_s}{d\ln\mu} = -2\epsilon\, a_s - 2a_s \sum_{i=0}^{\infty} a_s^{i+1}\beta_i\,, \text{with } \epsilon = (4-d)/2\,, \tag{9}$$

it is easy to express the renormalization constants Z in terms of anomalous dimensions γ order by order in $a_s = (\alpha_s)/(4\pi)$. Then one can extract the anomalous dimensions from the renormalization constants in the single pole of ϵ:

$$Z|_{1/\epsilon} = \sum_{l=1}^{\infty} a_s^l \frac{1}{l\,\epsilon}\gamma^{(l-1)}\,. \tag{10}$$

In the rest of this proceeding, we expand renormalization constants and anomalous dimensions in the following form,

$$Z = \sum_{l=0}^{\infty} a_s^l Z^{(l)}, \qquad \gamma = \sum_{l=1}^{\infty} a_s^l \gamma^{(l-1)}\,. \tag{11}$$

2. A general framework to renormalize the twist-two operators

When considering the off-shell OMEs with a twist-two operator insertion, equation (5) needs to be extended, i.e. the physical operators O_q and O_g could mix with unknown gauge-variant (GV) operators under renormalization. This mixing was already pointed out by Gross and Wilczek in the first calculation of singlet anomalous dimensions [20]. To find the unknown GV operators to renormalize the twist-two operators, there is great progress in the literature [21–26]. However, the problem is never completely solved. Recently, starting from a generalized BRST symmetry, Falcioni and Herzog [27] proposed a method enabling the construction of the GV operators for fixed n to higher orders of strong coupling constants. It remains quite challenging to obtain high-n operators.

In [28], we proposed a new method that enables the determination of GV counterterms with full-n dependence. We first explain the basic idea of the new method. By computing the off-shell OMEs with the insertion of bare operators O_q^{B}, O_g^{B}, and combing them according to the renormalization procedure on the right-hand side of equation (5), we observed that the two-by-two mixing matrix is not enough to make the right-hand side finite. It is then natural to introduce some extra GV operators (counterterms) to cancel the remaining divergences. Therefore, the new renormalization procedure reads

$$\begin{pmatrix} O_q \\ O_g \\ O_{ABC} \end{pmatrix}^{\mathrm{R}} = \begin{pmatrix} Z_{qq} & Z_{qg} & Z_{qA} \\ Z_{gq} & Z_{gg} & Z_{gA} \\ 0 & 0 & Z_{AA} \end{pmatrix} \begin{pmatrix} O_q \\ O_g \\ O_{ABC} \end{pmatrix}^{\mathrm{B}} + \begin{pmatrix} [ZO]_q^{\mathrm{GV}} \\ [ZO]_g^{\mathrm{GV}} \\ [ZO]_A^{\mathrm{GV}} \end{pmatrix}^{\mathrm{B}}, \tag{12}$$

where we introduce the GV operator $O_{ABC} = O_A + O_B + O_C$ with O_A, O_B, O_C denoting the pure-gluon, quark-gluon, and ghost-gluon GV operators respectively. At higher orders of a_s, in addition to the GV operator O_{ABC}, three GV counterterms $[ZO]_q^{\mathrm{GV}}$, $[ZO]_g^{\mathrm{GV}}$, $[ZO]_A^{\mathrm{GV}}$ are also required to renormalize the physical twist-two operators. For GV counterterms, Z and O are written together for the reason that it becomes impossible to disentangle the renormalization constants Z from their associated operators O while retaining the complete dependence on all powers of n. Notice that the subscript i in GV counterterm $[ZO]_i^{\mathrm{GV}}$ is just a name with respect to the renormalization of O_i operator. Each GV counterterm $[ZO]_i^{\mathrm{GV}}$ could involve pure-gluon, quark-gluon, and ghost-gluon GV counterterms. The GV counterterms can be expanded formally as the following form

$$[ZO]_i^{\mathrm{GV}} = \sum_l^{\infty} a_s^l \, [ZO]_i^{\mathrm{GV},\,(l)}, \text{with } i = q, g, A\,. \tag{13}$$

The GV operators or counterterms only start to contribute from specific orders of a_s,

$$\begin{aligned} Z_{qA} = \mathcal{O}(a_s^2), \quad Z_{gA} = \mathcal{O}(a_s), \quad [ZO]_q^{\mathrm{GV}} = \mathcal{O}(a_s^3), \quad [ZO]_g^{\mathrm{GV}} = \mathcal{O}(a_s^2), \\ Z_{AA} = \mathcal{O}(a_s^0), \quad [ZO]_A^{\mathrm{GV}} = \mathcal{O}(a_s)\,. \end{aligned} \tag{14}$$

Up to now, we know very little about the form of GV operator O_{ABC} or counterterms $[ZO]_i^{\mathrm{GV}}$. In the following, we extract more information for them. As an example, it is sufficient to consider the renormalization of the operator O_g:

$$O_g^{\mathrm{R}} = Z_{gq} O_q^{\mathrm{B}} + Z_{gg} O_g^{\mathrm{B}} + Z_{gA} O_{ABC}^{\mathrm{B}} + [ZO]_g^{\mathrm{GV}}\,. \tag{15}$$

The idea is to insert the above equation into matrix elements with specific off-shell external states. Due to the property of twist-two operators, it is sufficient to consider the following one-particle-irreducible (1PI) OMEs with all-off-shell external states consisting of two particles of type j plus

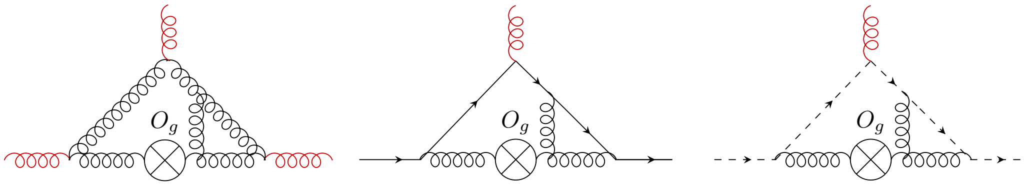

Figure 1: Sample 2-loop Feynman diagrams to determine the counterterm Feynman rules with 3 legs stemming from $[ZO]_g^{\mathrm{GV},(2)}$.

m gluons,

$$\langle j|O_g|j+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,\mathrm{R}} = Z_j(\sqrt{Z_g})^m\Bigg[\langle j|(Z_{gq}O_q+Z_{gg}O_g)|j+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,\mathrm{B}}\Bigg]$$
$$+Z_j(\sqrt{Z_g})^m\Bigg[Z_{gA}\,\langle j|O_{ABC}|j+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,\mathrm{B}}+\langle j|[ZO]_g^{\mathrm{GV}}\,|j+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,\mathrm{B}}\Bigg]\,. \qquad (16)$$

Here, j denotes quarks(q), gluons(g), or ghosts(c) and $\sqrt{Z_j}$ is the corresponding field renormalization constant. To make the extraction of (counterterm) Feynman rules transparent, we expand the off-shell OMEs according to the number of loops l and legs $m+2$,

$$\langle j|O|j+m\,g\rangle^{\mu_1\cdots\mu_m} = \sum_{l=1}^{\infty}\left[\langle j|O|j+m\,g\rangle^{\mu_1\cdots\mu_m,(l),(m)}\right]a_s^l\,g_s^m\,. \qquad (17)$$

Due to the hierarchy of GV operators (counterterms) shown in equation (14), one can extract the GV (counterterm) Feynman rules by computing the off-shell OMEs order by order in the strong coupling constant. For example, the Feynman rules for O_C operator with two-ghost plus m gluons can be written in the following simple form,

$$Z_{gA}^{(1)}\,\langle c|O_C|c+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,(0),(m)} = -\left[\langle c|O_g|c+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,(1),(m),\mathrm{B}}\right]_{\mathrm{div}}, \qquad (18)$$

where the subscript 'div' is the pole part in dimensional regulator ϵ, and we only need to consider one-loop OMEs. Similarly, the two-loop counterterm Feynman rules of $[ZO]_g^{\mathrm{GV},(2)}$ with two-ghost plus m gluons can be written as:

$$\begin{aligned}\langle c|[ZO]_g^{\mathrm{GV},(2)}\,|c+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,(0),(m)} &= -\Bigg\{\Bigg[\,\langle c|O_g|c+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,(2),(m),\mathrm{B}}\\
&+\left(Z_c^{(1)}+\frac{mZ_g^{(1)}}{2}+Z_{gg}^{(1)}-\frac{\beta_0(m+2)}{2\epsilon}\right)\langle c|O_g|c+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,(1),(m),\mathrm{B}}\\
&+\left(Z_c^{(1)}Z_{gA}^{(1)}+\frac{1}{2}mZ_g^{(1)}Z_{gA}^{(1)}-\frac{\beta_0 mZ_{gA}^{(1)}}{2\epsilon}+Z_{gA}^{(2)}\right)\langle c|O_C|c+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,(0),(m),\mathrm{B}}\\
&+Z_{gA}^{(1)}\,\langle c|O_{AC}|c+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,(1),(m),\mathrm{B}}\\
&+Z_g^{(1)}\sum_{t=1}^{s}\xi^t\,t\,\langle c|O_g|c+m\,g\rangle_{\mathrm{1PI}}^{\mu_1\cdots\mu_m,(1),(m),(t),\mathrm{B}}\Bigg]_{\mathrm{div}}\Bigg\}\Bigg|_{\xi^{\mathrm{B}}\to\xi}\,, \qquad (19)\end{aligned}$$

where ξ is the gauge parameter with $\xi=1$ in Feynman gauge. Other (counterterm) Feynman rules can also be written down similarly. We show some sample diagrams of determining two-loop

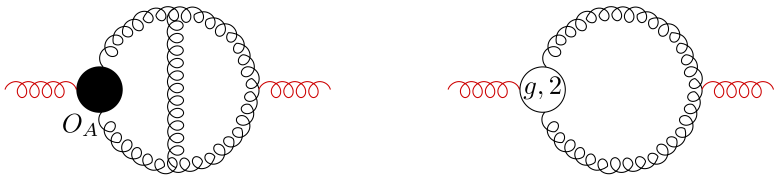

Figure 2: Sample diagrams with the insertion of GV operator O_A or two-loop GV counterterm $[ZO]_g^{\mathrm{GV},(2)}$, they enter the calculations of splitting functions starting from three-loop order.

counterterm Feynman rules in Fig. 1. We noticed that the framework shown above is general and works for any number of loops and legs.

3. Computational methods

In the previous section, we presented a general framework to renormalize the physical twist-two operators. The challenge of determining required GV (counterterm) Feynman rules is transformed into the computations of off-shell multi-loop multi-leg OMEs. Upon acquiring these (counterterm) Feynman rules, they can be inserted into multi-loop matrix elements involving two legs. By computing the off-shell multi-loop two-leg OMEs with the insertion of physical operators as well as GV (counterterm) operators, one can derive the anomalous dimensions or splitting functions to high loop order. Some sample diagrams with the insertion of GV operator O_A or two-loop counterterms can be found in Fig. 2.

To keep the full-n dependence for the off-shell OMEs, we adopted a generation function method first proposed in [29, 30]. The method sums the non-standard terms like $(\Delta \cdot p)^{n-1}$ into linear propagators depending on a tracing parameter t. As an example,

$$(\Delta \cdot p)^{n-1} \to \sum_{n=1}^{\infty} (\Delta \cdot p)^{n-1} t^n = \frac{t}{1 - t\Delta \cdot p}\,. \tag{20}$$

We work in parameter-t space throughout and extract the n-space results at the final stages by expanding the parameter t around $t = 0$. The computational steps follow a standard chain, including generations of diagrams and unreduced amplitude, reducing the amplitude using integration-by-parts identities [31–33], solving the master integrals by (canonical) differential equations [34, 35], and so on. The computations were done with the help of different tools, for example, `QGRAF` [36], `FORM` [37], `Reduze 2` [38], `FeynCalc` [39, 40], `Apart` [41], `MultivariateApart` [42], `Singular_pfd` [43], `LiteRed` [44], `FIRE6` [45], `Kira` [46], `CANONICA` [47, 48], `Libra` [49, 50], `FiniteFlow` [51], `HarmonicSums` [52–57], `HPL` [58] as well as a private code `Finred` by Andreas von Manteuffel based on finite field sampling and rational reconstruction [51, 59, 60].

4. Results

With the methods presented above, in [28] we had determined the Feynman rules resulting from operator O_{ABC} to g_s^2, as well as the counterterm Feynman rules resulting from counterterm

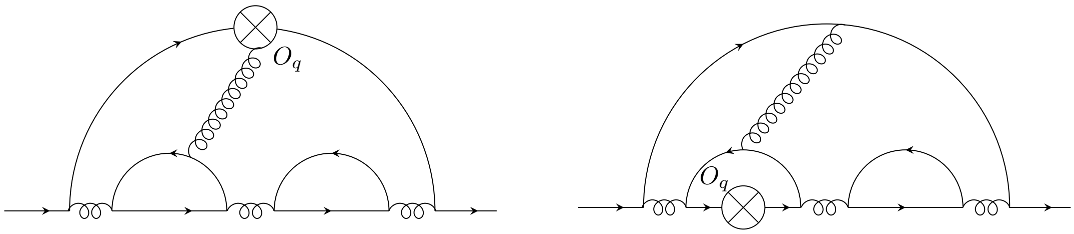

Figure 3: Representative Feynman diagrams for N_f^2 contributions to the OME $\langle q|O_q^{\mathrm{B}}|q\rangle$ at four loops. The first diagram contributes to the non-singlet anomalous dimension, while the second diagram contributes to the pure-singlet anomalous dimension in the quark channel.

operator $[ZO]_g^{\mathrm{GV}}$ to $a_s^2\, g_s$, where a_s^2 is from Z and g_s is from O. Similarly with the Feynman rules for physical operators O_q, O_g, the Feynman rules for operator O_{ABC} were found to involve only multiple summations like $\sum_{j=0}^{n-3}(\Delta\cdot p_1)^{n-3-j}(\Delta\cdot p_2)^j$. However, the counterterm Feynman rules at order $a_s^2\, g_s$ for $[ZO]_g^{\mathrm{GV}}$ exhibit a complicated pattern, which involve transcendental functions: harmonic sums [61, 62] as well as generalized harmonic sums [63], for example

$$S_{1,1}\left(1, z_1+1; n\right) = \sum_{t_1=1}^{n}\frac{1}{t_1}\sum_{t_2=1}^{t_1}\frac{(1+z_1)^{t_2}}{t_2}\,,\ \text{with}\ z_1 = \frac{\Delta\cdot p_2}{\Delta\cdot p_1}\,. \tag{21}$$

Based on the computations of off-shell OMEs, the above (counterterm) Feynman rules enable us to determine the three-loop splitting functions for all channels in the unpolarized singlet sector. In the non-singlet sector, the GV operators (counterterms) are absent, and the first three-loop calculations based on off-shell OMEs were presented in [64]. We repeated the calculation in our convention and found full agreement with them. The obtained three-loop singlet and non-singlet splitting functions agree with the results [4, 5] extracted from forward deep inelastic scattering.

In [10], we found the same (counterterm) Feynman rules are enough to extract the four-loop $q\to q$ splitting functions. We determined the four-loop pure-singlet splitting functions involving two closed quark loops for the first time in the same paper [10]. Some sample diagrams can be found in Fig 3. By evaluating the corresponding anomalous dimensions with full-n dependence at fixed-n values, we cross-validated our result against the fixed-n result up to $n=20$ shown in [12].

To go beyond the N_f^2 contributions, in [16] we computed the $N_f\,C_F^3$ contribution to four-loop non-singlet splitting functions for the first time. Some sample Feynman diagrams can be found in Fig. 4. The GV operators (counterterms) are not required in this case. The corresponding anomalous dimension successfully passes the check against the results with fixed moments to $n=16$ [9].

All partially known splitting functions at four-loop order can be expressed solely in terms of harmonic polylogarithms [65]. It will be interesting to see if we need generalized polylogarithms or even special functions beyond generalized polylogarithms to express the full results at the four-loop order.

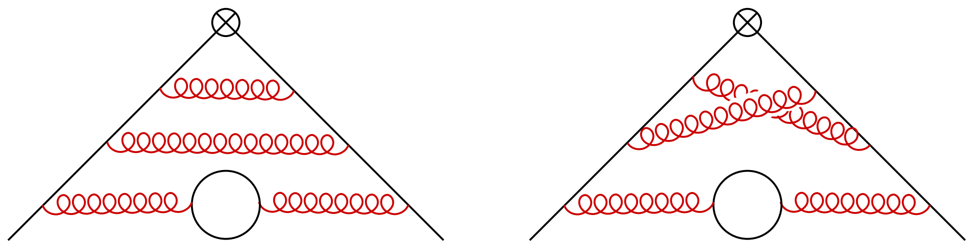

Figure 4: Sample Feynman diagrams for the $N_f C_F^3$ contribution to the four-loop, non-singlet OME with two external quarks. The crossed circle represents the non-singlet operator $O_{\rm ns}$.

5. Conclusions

When considering the off-shell OMEs with a twist-two operator insertion, the physical operators O_q, O_g mix with the priority unknown gauge-variant operators. We proposed a general framework to systematically determine the full-n (counterterm) Feynman rules stemming from those gauge-variant (counterterm) operators. The derived (counterterm) Feynman rules allow us to determine the three-loop singlet splitting functions based on the off-shell operator matrix element method, for the first time. The same (counterterm) Feynman rules also enable the determination of the new result for four-loop pure-singlet splitting functions with two closed fermionic loops. We also computed the first $N_f C_F^3$ contributions to the four-loop non-singlet splitting functions, where the gauge-variant counterterms are not required.

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