How to achieve precise perturbative prediction from a fixed-order calculation?

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The intrinsic conformality is a general property of the renormalizable gauge theory, which ensures the scale-invariance of a fixed-order perturbative series at each perturbative order. In the paper, following the idea of intrinsic conformality, we suggest a novel single-scale setting approach under the principal of maximum conformality (PMC) to remove the conventional renormalization scheme-and-scale ambiguities. We call this newly suggested single-scale procedure as the PMC\(_{\infty}\)-s approach, in which an overall effective strong coupling constant, and hence an overall effective scale is achieved by identifying the \(\{\beta_0\}\)-terms at each order. Its resultant conformal series is scale-invariant and satisfies all the renormalization group requirements. The PMC\(_{\infty}\)-s approach is applicable to any perturbatively calculable physical observables, and its resultant perturbative series provides an accurate basis for estimating the contribution from the unknown higher-order (UHO) terms. By using the Higgs decays into two gluons up to five-loop QCD corrections as an example, we show how the PMC\(_{\infty}\)-s works, and we obtain \(\Gamma_{H}^{\text{PAA}}\)\(_{\text{PMC}_{\infty}}\) = 334.45\(\pm\)2.07 KeV and \(\Gamma_{H}^{\text{B.A.}}\)\(_{\text{PMC}_{\infty}}\) = 334.45\(\pm\)6.34 KeV, where the errors mentioned in the body of the text have added in quadrature and the Padé approximation approach (PAA) and Bayesian approach (B.A.) have been adopted to estimate the contributions from the UHO-terms, respectively. We also demonstrate that the PMC\(_{\infty}\)-s approach is equivalent to the previously suggested single-scale setting approach (PMCs), which also follows from the PMC but treats the \(\{\beta_i\}\)-terms from different point of view. Thus a proper using of the renormalization group equation can provide a solid way to solve the scale-setting problem.

I. INTRODUCTION

Due to its asymptotic freedom property \([1, 2]\), the QCD running coupling becomes numerically small at short distances, allowing perturbative calculations of cross sections or decay widths for high momentum transfer processes. To yield finite and reliable expressions for perturbatively calculable observables, one needs to regulate and cancel the divergences that occur commonly in perturbation theory calculations. For the purpose, certain renormalization scheme and renormalization scale have to be introduced to finish the renormalization procedures. As the requirement of renormalization group invariance (RGI), a valid prediction for a physical observable must be independent to any choices of renormalization scheme and renormalization scale. However a truncated perturbation series does not automatically satisfy these requirements. The approach of using a guessed renormalization scale and choosing an arbitrary range for its uncertainty is conventional, which however leads to renormalization scheme-and-scale ambiguities and greatly depresses the predictive power of perturbative QCD (pQCD) theory.

One may hope to achieve a scheme-and-scale independent prediction by systematically computing higher-order enough QCD corrections; however, this hope is in conflict with the presence of the divergent \(n! \alpha_s^n \beta_0^n\) renormalon series. The complication of a higher-order loop calculation increases greatly with the number of loops as well as the number of external legs. It is thus important to find a proper way to achieve precise information as much as possible from the known perturbative series. The renormalization scale-setting problem then becomes one of the most important problems for achieving precise fixed-order pQCD predictions \([3]\).

In the literature, the principle of maximum conformality (PMC) \([4–8]\) has been suggested to eliminate the conventional renormalization scale-and-scheme ambiguities. The \(\alpha_s\)-running behavior is governed by the renormalization group equation (RGE): Then the \(\{\beta_i\}\)-terms emerged in perturbative series can be inversely adopted for fixing the correct value of \(\alpha_s\) for a physical observable. The key point of PMC is to rightly fix the magnitude of \(\alpha_s\) by using the RGE recursively, which also provides a solid way to extend the well-known Brodsky-Lepage-Mackenzie (BLM) approach \([9]\) to all orders. It has been demonstrated that the PMC prediction is independent to any choice of renormalization scale and scheme \([10]\), being consistent with the fundamental renormalization group approaches \([11–15]\) and the self-consistency requirements of the renormalization group \([16]\).

The PMC was initially introduced as a multi-scale-setting approach \([4–8]\), in which distinct PMC scales at each order are determined by using different categories of the \(\{\beta_i\}\)-terms at the corresponding orders. Because of it’s perturbative nature, the resultant PMC scale-invariant series still has two kinds of residual scale depen-
ence due to unknown higher-order (UHO) terms [17]; i.e., the last perturbative terms of the PMC scales are unknown (first kind of residual scale dependence), and the last perturbative terms of the pQCD approximant are not fixed since its PMC scale cannot be fixed (second kind of residual scale dependence). Even though, these two residual scale dependence are suppressed at high orders in $\alpha_s$ and/or from exponential suppression, if the convergence of the perturbative series of either the PMC scale or the pQCD approximant is weak, such residual scale dependence could be significant. As a step forward, it is helpful to find proper way to suppress the residual scale dependence of the PMC predictions.

It has been found that the intrinsic conformality (iCF), which ensures the scale-invariance at each order by only identifying the $\{\beta_0\}$-terms at each order, could be helpful to suppress the residual scale dependence. By taking iCF into account, an infinity-order scale-setting approach called as the PMC$_\infty$ approach [18] has been proposed. In the literature, Ref. [19] suggests another alternative PMC multi-scale-setting procedure (PMCa), whose effective scales are fixed by requiring all the scale-dependent terms at each order vanish. It has been shown that PMCa and PMC$_\infty$ approaches are equivalent to each other [20]. This equivalence reflects the fact that the iCF requires the scale invariance of the pQCD series at each order, and vice versa. Some applications of PMC$_\infty$ can be found in Refs. [21, 22]. It is however still a multi-scale-setting approach, even though the newly determined PMC scales at each orders are free of first kind of residual scale dependence, it still has the second kind of residual scale dependence, which may be sizable for lower-order predictions. And it may meet very small scale problem at some specific orders [20]. Towards the goal of achieving minimum scale-dependent prediction, following the idea of iCF, in this paper, we shall introduce a novel single-scale approach (named PMC$_\infty$-s) to set an overall effective scale of the process, which shall also be helpful to estimate the contribution from the UHO-terms. We shall show that it also fixes the conventional renormalization scale ambiguity and provides further suppression to the residual scale dependence.

The idea of single-scale setting approach has been initially suggested in Refs. [23, 24] by applying the BLM approach, whose purpose at that time is to extend the BLM to higher-orders, e.g. the two-loop level. Lately, it has been found that by transforming the $n_f$-series into $\{\beta_i\}$-series correctly with the help of RGE, an all-orders single-scale approach by using the PMC (named PMCs) can be achieved [25]. It has been shown that the PMCs approach can serve as a reliable substitute for the full multi-scale PMC approach, and that it does lead to more precise pQCD predictions with less residual scale dependence, cf. Refs. [10, 20] and references therein. The PMCs also provides a self-consistency way to achieve precise $\alpha_s$ running behavior in both the perturbative and nonperturbative domains [26, 27]. It is thus interesting to show what’s the relation between the PMC$_\infty$-s and the PMCs approaches. Moreover, by using the scale-invariant PMC$_\infty$-s series, we adopt two approaches to estimate the contributions from the unknown higher-order terms, which are important to extend the predictive power of the pQCD theory.

The remaining parts of this paper are organized as follows. We give the PMC$_\infty$-s approach in Sec. II, a demonstration of its equivalence to PMCs is also given there. As an explicit application, we then apply PMC$_\infty$-s approach to deal with the decay width of the Higgs decays into two gluons. Numerical results and discussions are given in Sec. III. Sec. IV is reserved for a summary.

II. CALCULATION TECHNOLOGY

The $\alpha_s$-running behavior is governed by the following standard RGE,

$$
\beta(a_s(\mu_r)) = \mu_r^2 \frac{d a_s(\mu_r)}{d \mu_r^2} = -a_s^2(\mu_r) \sum_{i=0}^{\infty} \beta_i a_s^i(\mu_r),
$$

(1)

where the right-hand-side is a perturbative expansion in terms of $a_s = \alpha_s / 4\pi$. By using the RGE, one can fix the $\alpha_s$ value at any perturbative scale by using the measurements of high-energy observables that can fix the coupling at a given scale such as $M_2$. The $\{\beta_i\}$-functions have been known up to five-loop level in the modified minimal-subtraction scheme (\overline{MS} scheme) [28–36].

By using the Taylor expansion, one can derive a scale-displacement relation of the couplings at two different scales $\mu_1$ and $\mu_2$,

$$
a_s^k(\mu_2) = a_s^k(\mu_1) + \sum_{n=1}^{\infty} (-1)^n \Theta_k^{(n)}(a_s(\mu_1)) \ln^n \frac{\mu_2^2}{\mu_1^2},
$$

(2)

where we have introduced the notation

$$
\Theta_k^{(n)}(a_s(\mu_1)) = \frac{1}{n!} \left( \frac{d^n a_s^k(\mu_1)}{d \mu_1^2} \right)_{\mu_1=\mu_2}. \tag{3}
$$

We thus have

$$
\Theta_k^{(1)}(a_s(\mu_r)) = k a_s^{k-1} \beta,
$$

$$
\Theta_k^{(2)}(a_s(\mu_r)) = \frac{1}{2!} k a_s^{k-1} \beta \left[ (k-1) \frac{\beta}{a_s} + \frac{d \beta}{da_s} \right],
$$

$$
\Theta_k^{(3)}(a_s(\mu_r)) = \frac{1}{3!} k a_s^{k-1} \beta \left[ (k-1)(k-2) \frac{\beta^2}{a_s^2} + (k-1) \frac{d \beta}{a_s} \left( \frac{d \beta}{da_s} \right) + \frac{d^2 \beta}{da_s^2} \right],
$$

$$
\cdots.
$$

A. The newly suggested PMC$_\infty$-s approach

Generally, a pQCD calculable physical observable $\rho$ can be written as

$$
\rho = \sum_{i=1}^{p} L_i(\mu_r, Q) a_s^{n+i-1}(\mu_r),
$$

(4)
where $n$ is the $\alpha_s$-power of the leading-order terms, $\mu_r$ is the renormalization scale, $Q$ represents the kinematic scale at which the observable is measured or the typical momentum flow of the process, and

$$\mathcal{L}_i(\mu_r, Q) = \sum_{j=0}^{i-1} c_{i,j}(\mu_r, Q) n_j^r$$

is the perturbative coefficients with $n_f$ being the number of active light-quark flavors. When the sum is over all perturbative terms, corresponding to $p \to \infty$, the physical observable shall be independent to any choice of $\mu_r$ due to the cancellation of $\mu_r$-dependence among all the perturbative terms. While for a fixed-order prediction, one needs to be careful about the scale-setting problem.

One can further separate the perturbative coefficients $\mathcal{L}_i$ into the scale-invariant iCF ones $\mathcal{L}_{i,IC}(Q)$ and the scale-dependent ones $\mathcal{L}_i(\mu_r, Q)$, i.e.

$$\mathcal{L}_i(\mu_r, Q) = \mathcal{L}_{i,IC}(Q) + \mathcal{L}_i(\mu_r, Q).$$

The first IC coefficient $\mathcal{L}_{1,IC}$ equals to $\mathcal{L}_1$; the second IC coefficient $\mathcal{L}_{2,IC}$ can be derived by setting $n_f \equiv 33/2$ to the RGE-involved $n_f$-terms in $\mathcal{L}_2$ such that to remove the non-conformal contribution from the NLO-terms, $\mathcal{L}_{2,IC} = \mathcal{L}_2|_{n_f=33/2}$; etc. The perturbative series of $\rho$ under different choices of scale can be related by using the RGE, e.g. its series at any other scale can be derived from its perturbative series at $\mu_r = Q$. Then Eq.(4) can be reorganized as the following form,

$$\rho = \sum_{i=1}^{P} \mathcal{L}_{i,IC}(Q) a_s^{n+i-1}(Q_r) + \sum_{i=1}^{P} \sum_{j=1}^{P} (-1)^j \mathcal{L}_i(Q, Q) \Theta_{n+i-1}^j (a_s(\mu_r)) \ln \frac{Q_r^2}{Q^2},$$

where the scale-dependent log-terms have been explicitly written. Applying the RGE (1), or equivalently the scale-dependent relation (2), to Eq.(6), we then obtain

$$\rho = \sum_{i=1}^{P} \mathcal{L}_{i,IC}(Q) a_s^{n+i-1}(Q_s) + \sum_{i=1}^{P} \mathcal{L}_i(Q, Q) a_s^{n+i-1}(Q_s) + \sum_{i=1}^{P} \sum_{j=1}^{P} (-1)^j \mathcal{L}_i(Q, Q) \Theta_{n+i-1}^j (a_s(Q_s)) \ln \frac{Q_s^2}{Q^2},$$

which is free of $\mu_r$-dependence and is equivalent to set $\mu_r = Q_s$ in Eq.(6) directly. This shows that if the value of scale $Q_s$ is fixed by requiring all the non-conformal terms or explicitly the last two summing terms in the right-hand-side of Eq.(7) to vanish, we shall get the required scale-invariant pQCD series, well satisfying the property of iCF. We call the above scale-setting procedures as the PMC$_\infty$-s approach, which only needs to fix one overall effective scale $Q_s$ and results in the following scale-invariant series,

$$\rho = \sum_{i=1}^{P} \mathcal{L}_{i,IC}(Q_s) a_s^{n+i-1}(Q_s).$$

(8)

It shows that the PMC$_\infty$-s approach solves the conventional $\mu_r$-dependence, and it also removes the second kind of residual scale dependence. To determine the magnitude of $Q_s$, it is convenient to fix the value of $\ln \frac{Q_s^2}{Q^2}$, which can be expanded as a perturbative series

$$\ln \frac{Q_s^2}{Q^2} = \sum_{k=0}^{\infty} S_k a_s^k(Q_s) = \sum_{k=0}^{\infty} F_k a_s^k(Q_0).$$

(9)

Due to the perturbative nature of $\ln \frac{Q_s^2}{Q^2}$, the PMC$_\infty$-s approach recovers the first residual scale dependence occurred in PMC original multi-scale approach [4–8], which however shall be highly suppressed, e.g. its magnitude is at the $O(a_s^{n+p+1})$-order level for a given $(n+p)$th-order fixed-order series, or more specifically, the first kind of residual scale dependence is at the order of $\mathcal{O}\left( \left( \sum_{i=1}^{P} \mathcal{L}_{i,IC}(Q) a_s^{i-1}(Q_s) \right) O(a_s^{n+p+1}) \right)$. The first equality of Eq.(9) stands for the exact solution which can be solved numerically. Practically, one can expand the series over a critical coupling $a_s(Q_0 \sim Q)$ up to the required order such that the difference between the expansion over $a_s(Q_0)$ and the exact one is less than 1% or 0.1%. Then, if the right-hand-side series is convergent or the scale $Q_0$ is large enough such that the strong coupling $\alpha_s(Q_0) \ll 1$, we can adopt the second equality as the basis to do the analysis [25]. The coefficients $S_i$ or $F_i$ up to next-to-⋯-to-leading-log ($N^\infty$LL) accuracy can be determined by a $N^{n+1}$LO pQCD calculation. The expressions of the iCF coefficients $\mathcal{L}_{i,IC}$, $S_i$ and $F_i$ up to five-loop QCD corrections, and the relations between $S_i$ and $F_i$ are given in the
Appendix for convenience. In addition to the standard fixing of iCF coefficients $\mathcal{L}_{i, 1C}(Q)$, the above solution also implies another way of setting the iCF coefficients, e.g.

$$
\sum_{i=1}^{p} (\mathcal{L}_{i, 1C}(Q) - \mathcal{L}_{i}(Q, Q)) a_s^{n+i-1}(Q_s) = \sum_{i=1}^{p} \sum_{j=1}^{p} (-1)^j \mathcal{L}_{i}(Q, Q) \Theta_{n+i-1}^{(j)} (a_s(Q_s)) \left( \sum_{k=0}^{p-2} S_k a_s^k(Q_s) \right)^j.
$$

(10)

B. Equivalence of the PMC$_\infty$-s and the PMC-s approaches

In the literature, the PMCs approach also provides an all-orders single-scale approach to fix the conventional renormalization scale ambiguity [25]. Though their starting points are quite different, in the following, we shall show that the PMCs and the PMC$_\infty$-s approaches are in fact equivalent to each order. For the purpose, we first give a brief introduction of the PMCs approach. It first adopts the standard RGE and the degeneracy relations among different orders [37] to transform the RG-involved $n$-series into the $\{\beta_i\}$-series, i.e. Eq.(4) can be written as the following form,

$$
\rho = r_{1,0} a_s^0(\mu_r) + [r_{2,0} + n \beta_0 r_{2,1}] a_s^{n+1}(\mu_r) + \left[ r_{3,0} + n \beta_1 r_{2,1} + (n+1) \beta_0 r_{3,1} + \frac{n(n+1)}{2} \beta_0^2 r_{4,2} \right] a_s^{n+2}(\mu_r)
$$

$$
+ \left[ r_{4,0} + n \beta_2 r_{2,1} + (n+1) \beta_1 r_{3,1} + \frac{n(n+1)(n+2)}{2} \beta_0 \beta_1 r_{3,2} + (n+2) \beta_0 r_{4,1} + \frac{(n+1)(n+2)}{2} \beta_0^2 r_{4,2} \right] a_s^{n+3}(\mu_r)
$$

$$
+ \left[ r_{5,0} + n \beta_3 r_{2,1} + (n+1) \beta_2 r_{3,1} + \frac{n(n+2)}{2} (\beta_1^2 + 2 \beta_1 \beta_0) r_{3,2} + \frac{(n+1)(n+2)}{2} (2 \beta_2 r_{4,1} + (n+3) \beta_0 r_{5,1}) \right] a_s^{n+4}(\mu_r) + \cdots.
$$

(11)

The renormalization scale dependent perturbative coefficients $r_{i,j}$ can be redefined as

$$
| = C_j^k \rho_{i-k,j-k} \ln^k \frac{\mu_r^2}{Q^2},
$$

(12)

where $C_j^k = j! / (k!(j-k)!)$ are combination coefficients, and $\rho_{i,j} = r_{i,j}|_{\mu_r=0}$, specially, $\rho_{i,0} = r_{i,0}$. Then following the standard procedures of the PMCs, all the non-conformal $\{\beta_i\}$-terms are resummed to fix an overall effective coupling $a_s(Q_s)$, and the $N^{p-1}$-LO-order qPQCD prediction with $\alpha_s^n$ for leading-order terms (11) changes to the following conformal series:

$$
\rho = \sum_{i=1}^{p} r_{i,0} a_s^{n+i-1}(Q_s).
$$

(13)

Similarly, to determine the magnitude of $Q_s$, we can expand $Q_s^2 / Q^2$ as a power series over $a_s(Q_s)$ [10]:

$$
\ln \frac{Q_s^2}{Q^2} = \sum_{k=0}^{p-2} T_k a_s^k(Q_s),
$$

(14)

which can be fixed up to $N^{p-2}$-LL-accuracy for a given $N^{p-1}$-LO-order qPQCD series. And after a careful calculation, we observe that

$$
\hat{r}_{i,0} = \mathcal{L}_{i,1C}, \quad (i = 1, 2, \cdots, p)
$$

(15)

and

$$
T_k = S_k, \quad (k = 0, 1, \cdots, p - 2).
$$

(16)

Thus the predictions using the PMC$_\infty$-s approach and the PMCs approach are overlap with each other. The explicit equivalence of the PMC$_\infty$-s and the PMCs formulas up to the case of $p = 5$ can be achieved by comparing Eqs.(60-73) with the PMCs formulas given in Refs.[10, 25]. The PMCs conformal series (13) satisfies the renormalization group invariance [38] and its prediction is scheme-and-scale independent.
### III. A NEW ANALYSIS OF THE HIGGS BOSON DECAYS INTO TWO GLUONS USING THE PMC SINGLE-SCALE APPROACH

The $H \to gg$ decay plays an important role in Higgs phenomenology. In this section, we take it as an explicit example to show that by using the PMC single-scale approach (PMC$_\infty$-s), a more accurate pQCD prediction can be achieved. Its total decay width $\Gamma_H$ up to N$^4$LO-level takes the form

$$\Gamma_H = \frac{5}{36\sqrt{2\pi}} \sum_{i=1}^{5} \frac{M_H^3 G_F}{s_i^{\frac{1}{2}}} \sum_{i=1}^{5} C_i(\mu_r) a_i^{(i+1)}(\mu_r), \quad (17)$$

where $i = (1, \cdots, 5)$ represents the LO-terms, the NLO-terms, ..., and the N$^4$LO-terms, respectively. The Fermi constant $G_F = 1.16638 \times 10^{-5}$ GeV$^{-2}$. The perturbative coefficients $C_{i\in[1,5]}(M_H)$ under the MS-scheme have been given in Refs. [39–48], which can be conveniently transformed to mMOM-scheme ones under the Landau gauge [49, 50].

To do the numerical calculation, we take [51], $M_H = 125.25 \pm 0.17$ GeV, $m_t = 172.76 \pm 0.30$ GeV and $\alpha_s(M_Z) = 0.1179 \pm 0.0009$.

#### A. Basic properties of the total decay width $\Gamma_H$ up to N$^4$LO QCD corrections

![Graph](image)

**FIG. 1:** The effective scale $Q_*$ up to LL, NLL, N$^2$LL, and N$^3$LL accuracies, respectively, which are numerically determined from Eq.(20) and are presented as the interactions.

Following the standard procedures of PMC$_\infty$-s, the above total decay width can be rewritten as

$$\Gamma_{H|\text{PMC}_{\infty}-s} = \frac{M_H^3 G_F}{36\sqrt{2\pi}} \sum_{i=1}^{5} C_{i\in[1,5]} a_i^{(i+1)}(Q_*), \quad (18)$$

where $C_{i\in[1,5]}$ are iCF coefficients which can be calculated by using Eqs.(60)–(64) listed in the Appendix, and the effective scale $Q_*$ can be determined up to N$^3$LL accuracy using the known N$^4$LO pQCD prediction, e.g.

$$\ln \frac{Q_*^2}{M_H^2} = S_0 + S_1 a_s(Q_*) + S_2 a_s^2(Q_*) + S_3 a_s^3(Q_*) \quad (19)$$

$$\begin{align*}
\ln \frac{Q_*^2}{M_H^2} &= -1.833 - 6.780 a_s(Q_*) - 906.753 a_s^2(Q_*) \\
&- 23279.302 a_s^3(Q_*),
\end{align*} \quad (20)$$

where all the input parameters have been set to be their central values. As shown by Fig.1, $Q_*$ can be fixed up to LL, NLL, N$^2$LL and N$^3$LL accuracies when $\Gamma_H$ has been known up to NLO, N$^2$LO, N$^3$LO and N$^4$LO levels, respectively. Numerically, we have

$Q_*^{\text{LL,NLL,N^2LL,N^3LL}} = \{50.081, 48.164, 45.266, 44.407\}$ GeV.

![Graph](image)

**FIG. 2:** Total decay width $\Gamma_H$ with different QCD corrections under conventional (Upper diagram) and PMC$_\infty$-s (Lower diagram) scale-setting approaches, respectively. The dashed line with cross symbols, the dotted line, the dash-dot line, the dashed line, and the solid line represent the LO, NLO, N$^2$LO, N$^3$LO and N$^4$LO total decay widths, respectively.

We present the total decay width versus the renormalization scale $\mu_r$ before and after applying the PMC$_\infty$-s in Fig.2, and the corresponding values for the total
and individual decay widths of the decay $H \rightarrow gg$ up to N$^3$LO QCD corrections are given in TABLE I. Fig. 2 and TABLE I show that, as expected, the renormalization scale dependence under conventional scale-setting approach becomes smaller-and-smaller when more-and-more loop terms have been known. For example, we obtain $\Gamma_H|_{\text{Conv.}} = 337.44^{+1.94}_{-1.33}$ KeV for the N$^4$LO-level prediction under the choice of $\mu_r \in [M_H/2, 2M_H]$, whose scale error is less than 1.0%. If taking a larger scale region, we shall have $\Gamma_H|_{\text{Conv.}} = 337.44^{+2.06}_{-1.33}$ KeV for $\mu_r \in [M_H/3, 3M_H]$, $\Gamma_H|_{\text{Conv.}} = 337.44^{+7.05}_{-1.33}$ KeV for $\mu_r \in [M_H/4, 4M_H]$, whose the net scale errors become slightly larger, e.g. 1.0% and 2.5%, respectively. Such small net scale dependence for the N$^4$LO prediction is due to good convergence of perturbative series and the cancellation of the scale dependence among different orders. The scale dependence for each loop terms are still large. To show this point more clearly, we define a $\kappa$ factor, $\kappa = \Gamma_H/\Gamma_{\text{LO}}$ to show the relative importance of each loop terms, and we have

$$\kappa|_{\text{PMC}_{\infty-s}} = 1 + 31.0\% - 17.3\% - 8.4\% + 1.4\%.$$
$$\kappa|_{\text{Conv.}} = 1 + 53.8^{+13.5}_{-15.0}\% + 6.6^{+15.7}_{-13.1}\% - 4.6^{+6.9}_{-2.2}\% - 1.6^{+0.6}_{-1.9}\%.$$

Here the PMCs prediction is scale invariant, which shows a good perturbative behavior and can be treated as the intrinsic perturbative nature of the pQCD approximant. The central values of conventional predictions are for $\mu_r = M_H$, which also has a good perturbative behavior due to the elimination of large log-terms which are always accompanied by the $\{\beta_i\}$-functions. However, the magnitudes of each loop terms of the conventional series are highly scale-dependent and the above errors are for $\mu_r \in [M_H/2, 2M_H]$. Since the decay widths do not monotonously increasing with the increment of scale, their upper limits are for $\mu_r = 2M_H$ and lower limits are for $\mu_r = 72.20$ GeV.

### B. An estimation of contributions from the uncalculated N$^3$LO terms

At present, remarkable progresses have been achieved in doing the higher-order calculations in perturbation theory. However due to the complexity of loop calculations, most of perturbatively calculable high-energy observables have only been calculated at lower-orders such as NLO, NNLO and etc. Thus it is important to have a way to estimate the possible contributions from the unknown higher-order terms (UHO-terms) such that to improve the predictive power of perturbative theory.

It has been conventional to take $\mu_r$ as the typical momentum flow ($Q$) of the process to obtain the central value of the pQCD series and to then vary $\mu_r$ within a certain range such as $[Q/2, 2Q]$ as a measure of a combined effect of scale uncertainties and the contributions from the UHO terms. The shortcomings of this treatment are apparent: It’s effectiveness heavily depends on the convergence of series which however usually will be diluted by the divergent renormalon terms; Each term in the perturbative series is highly scale-dependent and the net prediction does not satisfy the requirement of RGI; One only partly obtains the information of $\{\beta_i\}$-dependent UHO-terms which control the running of $\alpha_s$ and no information on the contributions from the conformal $\{\beta_i\}$-independent terms. For the more convergent and scale-invariant PMC$\infty-s$ series, it is expected that a much better prediction of UHO contributions can be achieved. For the purpose, we need to estimate the magnitude of the UHO-terms in the perturbative series of the pQCD approximant; and we also need to know the magnitude of the UHO-terms in the perturbative series of the PMC scale such that to have an estimation of the first kind of residual scale dependence.

Then the total uncertainty of a pQCD approximant due to the UHO-terms can be treated as the squared average of the predicted conventional scale dependence (or the first residual scale dependence) and the predicted magnitude of the UHO-terms in the perturbative series of the pQCD approximant.

In the following, we will first try two representative approaches to estimate the magnitude of the uncalculated N$^3$LO-terms for the total decay width $\Gamma_H$ by using the known N$^3$LO-level conventional and PMC$\infty-s$ series, respectively. The first approach is to directly predict the magnitude of the N$^3$LO-order UHO coefficient by using a fractional generating function whose parameters can be fixed by matching to the known N$^4$LO-order series, which is usually called as the Padé approximation approach (PAA) $[57–59]$. And the second approach is to quantify the UHO’s contribution in terms of a probability distribution whose representative treatment is to use the Bayes’ theorem, which is called as the Bayesian approach $[60–63]$. And then, we shall provide an estimation of the total uncertainty due to the UHO-terms.

### Table I: Total and individual decay widths (in unit: KeV) of the decay $H \rightarrow gg$ under conventional and PMC$\infty-s$ scale-setting approaches. As for conventional predictions, their central values are for $\mu_r = M_H$ and the errors are for $\mu_r \in [M_H/2, 2M_H]$.

| $\Gamma_i$ | $i = 1$, LO | $i = 2$, NLO | $i = 3$, N$^2$LO | $i = 4$, N$^3$LO | $i = 5$, N$^4$LO | Total |
|-----------|-------------|-------------|-------------|-------------|-------------|-------|
| $\Gamma_H|_{\text{Conv.}}$ | 218.66$^{+4.95}_{-4.96}$ | 116.62$^{+2.08}_{-10.67}$ | 14.44$^{+25.3}_{31.36}$ | $-8.70^{+13.84}_{-7.54}$ | $-3.57^{+1.74}_{-1.37}$ | 337.44$^{+1.94}_{-1.33}$ |
| $\Gamma_H|_{\text{PMC}_{\infty-s}}$ | 313.53 | 97.16 | $-54.18$ | $-26.42$ | 4.36 | 334.45 |
1. Estimation of $N^5$LO contributions using the Padé approximation approach

The PAA provides a systematic procedure for promoting a finite Taylor series to an analytic function. For the present known pQCD series (17) or (18), we can rewrite it as $\rho = a_s^2 \sum_{i=1}^{5} r_i a_s^{i-1}$, where $r_i = \frac{M_i^2 G_F}{36 \sqrt{2} \pi} C_i$ or $r_i C_i,IC$, respectively. Its $[N/M]$-type fractional generating function can be constructed as

$$\rho^{[N/M]}(Q) = a_s^2 b_0 + b_1 a_s + \cdots + b_N a_s^N$$

$$= \frac{a_s}{1 + c_1 a_s + \cdots + c_M a_s^M}$$

(23)

$$= \sum_{i=1}^{5} r_i a_s^{i+1} + r_6 a_s^7 + \cdots ,$$

(24)

where $M \geq 1$ and $N + M = 4$. The coefficients $b_i \in [0,N]$ and $c_i \in [1,M]$ can be expressed by using the coefficients $r_i \in [1,5]$. Thus the predicted $N^5$LO-coefficients $r_6$ under various $[N/M]$-types are

$$r_6^{[3/1]} = \frac{r_5^2}{r_4},$$

$$r_6^{[2/2]} = \frac{r_4^3 - 2 r_4 r_5 r_3 - 2 r_2^2}{r_5^2 - r_2 r_4},$$

$$r_6^{[1/3]} = \frac{1}{r_4} (r_4^3 - 3 r_4^2 r_3 - 2 r_1 r_5 r_3 + 2 r_2 r_5 r_3 + 2 r_4 r_3^2 + 3 r_2 r_4^2 + r_1 r_5^2 - 2 r_1 r_2 r_4),$$

$$r_6^{[0/4]} = \frac{1}{r_4} (r_4^3 - 2 r_2^2 r_4 + r_1^2 r_2^2 + r_1^2 r_3^2 + 3 r_1 r_3 r_2 - 2 r_1^2 r_3 r_2 + 2 r_1 r_3 r_2),$$

(25)

It has been observed that the diagonal $[2/2]$-type Padé series is preferable for estimating the unknown contributions from the conventional pQCD series [64, 65]; while the $[0/4]$-type one is preferable for the PMC series [66], which makes the PAA geometric series be self-consistent with the GM-L prediction [13].

Numerically, we obtain $C_6^{[2/2]} = (4.825^{+95.950}_{-60.060}) \times 10^7$ and $C_6^{[0/4]} = 7.919 \times 10^8$ for $\mu_r \in [M_H/2, 2 M_H]$. Then, the magnitudes of the $N^5$LO-level UHO-terms for the perturbative series (17) or (18) are

$$\Delta \Gamma_H^{N^5LO, UH, \mu_r}_{\text{Conv.}} = \pm \frac{M_3^3 G_F}{36 \sqrt{2} \pi} C_6(\mu_r) a_s^7(\mu_r) \bigg|_{\text{MAX}}$$

$$= \pm 2.32 \text{ KeV},$$

(26)

$$\Delta \Gamma_H^{N^5LO, UH, \mu_r}_{\text{PMC}_{\infty-s}} = \pm \frac{M_3^3 G_F}{36 \sqrt{2} \pi} C_6,IC(Q_s) a_s^7(Q_s)$$

$$= \pm 3.39 \text{ KeV},$$

(27)

where the subscript “MAX” stands for the maximum value within the chosen $\mu_r$-region. For conventional pQCD series, if a broader $\mu_r$-region such as $\mu_r \in [M_H/4, 4 M_H]$ has been taken, we have $C_6^{[2/2]} = (4.825^{+95.950}_{-60.060}) \times 10^7$, leading to a larger uncertainty, $\Delta \Gamma_H^{N^5LO, \mu_r}_{\text{Conv.}} = \pm 3.85 \text{ KeV}$. Since $\mu_r$ could be chosen arbitrarily, the scale-invariant PMC$_{\infty-s}$ series is a more accurate basis than the conventional scale-dependent one for estimating the UHO-contributions.

To estimate the first kind of residual scale dependence for the PMC$_{\infty-s}$ prediction (18), we first predict the unknown $N^4$LL-terms of the perturbative series (20) by using the same procedures of PAA, whose magnitude is $\pm \left| S_1^{[v/3]} a_s^2(Q_s^{N^4LL}) \right|$ with $S_1^{[v/3]} = -5.838 \times 10^5$. It leads to a scale shift, $\Delta Q_s = \pm 0.253 \text{ GeV}$, then the first kind of residual scale dependence becomes

$$\Delta \Gamma_H^{N^5LO, UH, \mu_r}_{\text{PMC}_{\infty-s}} = \pm 0.65 \text{ KeV},$$

(28)

which is smaller than the above derived conventional scale dependence, e.g.

$$\Delta \Gamma_H^{N^5LO, UH, \mu_r}_{\text{Conv.}} = \pm 3.85 \text{ KeV}, \mu_r \in [M_H/2, 2 M_H]$$

$$\Delta \Gamma_H^{N^5LO, UH, \mu_r}_{\text{PMC}_{\infty-s}} = \pm 3.85 \text{ KeV}, \mu_r \in [M_H/4, 4 M_H]$$

By taking the above conventional scale dependence (29), (30), or the first residual scale dependence (28), and the predicted magnitudes of the UHO-terms (26, 27) in the perturbative series of the pQCD approximant into consideration, the total uncertainties caused by the UHO-terms for the conventional series are

$$\Delta \Gamma_H^{UH, \mu_r}_{\text{Conv.}} = \pm 3.85 \text{ KeV}, \mu_r \in [M_H/2, 2 M_H]$$

$$\Delta \Gamma_H^{UH, \mu_r}_{\text{PMC}_{\infty-s}} = \pm 3.85 \text{ KeV}, \mu_r \in [M_H/4, 4 M_H]$$

and for the PMC$_{\infty-s}$ series, it becomes

$$\Delta \Gamma_H^{UH, \mu_r}_{\text{PMC}_{\infty-s}} = \pm 3.45 \text{ KeV}.$$

(33)

2. Estimation of $N^6$LO contributions using the Bayesian approach

The Bayesian approach (B.A.) quantifies the contributions of the UHO-terms in terms of the probability distribution. The B.A. is a powerful method to construct probability distributions in which the Bayes’ theorem is applied to iteratively update the probability as new information becomes available. A detailed introduction of the B.A. and its combination with the PMC approach have been given in Ref. [67], so we will only present the results here, and the interested readers may turn to Ref. [67] for all the B.A. formulas.

To apply the B.A., we first transform the perturbation series (17), (18) and (19) over $a_s = \alpha_s / 4 \pi$ back to the ones over $\alpha_s$:

$$\Gamma_{\text{Conv.}} = \sum_{i=1}^{5} r_i(\mu_r) a_s^{i+1}(\mu_r),$$

(34)
\[
\Gamma_H|_{\text{PMC}_{\infty-s}} = \sum_{i=1}^{5} r_i,\alpha_{s}^{i+1}(Q_s),
\]

(35)

\[
\ln \frac{Q^2}{Q^2} = \sum_{i=0}^{3} S_i,\alpha_{s}^{i}(Q_s),
\]

(36)

where

\[
r_i(\mu_t) = \frac{1}{(4\pi)^{i+1}} \frac{M_H^i G_F}{36 \sqrt{2} \pi} C_i(\mu_t),
\]

(37)

\[
r_i,\alpha_{s} = \frac{1}{(4\pi)^{i+1}} \frac{M_H^i G_F}{36 \sqrt{2} \pi} C_i,\alpha_{s},
\]

(38)

\[
S_i = \frac{1}{(4\pi)^{i}} S_i,
\]

(39)

Because the known coefficients of the conventional pQCD series are scale-dependent at every orders, the B.A. can only be applied after one specifies the choices for the renormalization scale, thus introducing extra uncertainties for the B.A. On the other hand, the PMC_{\infty-s} conformal series is scale-independent, which then provides a more reliable basis for obtaining constraints on the predictions for the UHO contributions.

Following the standard B.A. procedures, we obtain the smallest 95.5% credible intervals (CIs) for the N^4LO coefficients \( r_6(\mu_t = M_H) \) and \( r_{6,\alpha_{s}} \), which are \( r_6(\mu_t = M_H) \in [-1.3569, 1.3569] \) and \( r_{6,\alpha_{s}} \in [-0.5624, 0.5624] \), respectively. Then, the error of \( \Gamma_H \) caused by the UHO-terms for the conventional series under the B.A. is

\[
\Delta \Gamma_H|_{\text{Conv}}^{\text{N^4LO}} = \pm 1.44 \text{ KeV.}
\]

(40)

If taking \( \mu_t \in [M_H/2, 2M_H] \), we have

\[
\Delta \Gamma_H|_{\text{Conv}}^{\text{N^4LO}} = (\pm 2.53) \text{ KeV,}
\]

(41)

which, by taking \( \mu_t \in [M_H/4, 4M_H] \), changes to

\[
\Delta \Gamma_H|_{\text{Conv}}^{\text{N^4LO}} = (\pm 14.07) \pm 2.63) \text{ KeV.}
\]

(42)

And for the PMC_{\infty-s} series, the error of \( \Gamma_H \) caused by the UHO-terms is scale-invariant and smaller, i.e.

\[
\Delta \Gamma_H|_{\text{PMC}_{\infty-s}}^{\text{N^4LO}} = \pm 1.30 \text{ KeV.}
\]

(43)

Secondly, we observe that the predicted smallest 95.5% CIs for the N^4LL-level coefficient \( S_4 \) of \( \ln Q^2/Q^2 \) is \( S_4 \in [-17.0331, 17.0331] \), which leads to a scale shift \( \Delta Q_s = (4.047, -0.248) \) GeV to the N^3LL-level scale \( Q_s^{\text{N^3LL}} = 44.407 \) GeV. Then the first kind of residual scale dependence of the PMC_{\infty-s} series under the B.A. becomes

\[
\Delta \Gamma_H|_{\text{PMC}_{\infty-s}}^{\Delta Q_s} = (\pm 0.64, -0.63) \text{ KeV.}
\]

(44)

Finally, by taking the above conventional scale dependence (29, 30), or the first residual scale dependence (44), and the predicted magnitudes of the UHO-terms (41, 42, 43) in the perturbative series of the pQCD approximant into consideration, the total uncertainties caused by the UHO-terms of the conventional series using B.A. are

\[
\Delta \Gamma_H|_{\text{Conv}}^{\text{UHO}} = (\pm 3.19, -2.94) \text{ KeV, } \mu_t \in [M_H/2, 2M_H] \]

(45)

\[
\Delta \Gamma_H|_{\text{Conv}}^{\text{UHO}} = (\pm 15.74, -2.94) \text{ KeV, } \mu_t \in [M_H/4, 4M_H]
\]

(46)

and for the PMC_{\infty-s} series, it becomes

\[
\Delta \Gamma_H|_{\text{PMC}_{\infty-s}}^{\text{UHO}} = (\pm 1.45, -1.44) \text{ KeV.}
\]

(47)

The error ranges estimated by using the PAA and B.A. for conventional series are close to each other. As shown by Fig.3, due to a sharp probability density distribution for the present known N^4LO-level PMC_{\infty-s} series, the B.A. error range is less than half of the PAA one. Fig.3 illustrates the characteristics of the posterior distribution: a symmetric plateau with two suppressed tails. The posterior distribution given by the Bayesian approach depends on the prior distribution, and as more and more loop terms become known, the probability shall be updated with less and less dependence on the prior; i.e., the probability density becomes increasingly concentrated (the plateau becomes narrower and narrower and the tail becomes shorter and shorter) as more and more loop terms for the distribution are determined.

C. Uncertainties due to \( \Delta M_H, \Delta m_t \) and \( \Delta \alpha_s(M_Z) \)

In addition to the errors caused by the UHO-terms, there are also errors caused by the input parameters \( M_H, m_t \) and \( \alpha_s(M_Z) \), e.g. \( \Delta M_H = \pm 0.17 \text{ GeV, } \Delta m_t = \pm 0.30 \text{ GeV, and } \Delta \alpha_s(M_Z) = \pm 0.0009 \) [51]. When discussing the errors from one parameter, the other parameters are set to be their central value. We obtain

\[
\Delta \Gamma_H|_{\text{Conv}}^{\Delta M_H} = (\pm 1.22, -1.21) \text{ KeV,}
\]

(48)
\[ \Delta \Gamma_H^{\alpha_s(M_Z)} = \pm 0.01 \text{ KeV}, \quad (49) \]
\[ \Delta \Gamma_H^{\alpha_s(M_Z)} = (\pm 6.27 \pm 6.26) \text{ KeV}, \quad (50) \]
\[ \Delta \Gamma_H^{\alpha_s(M_Z)} = (\pm 6.05 \pm 6.02) \text{ KeV}, \quad (51) \]
\[ \Delta \Gamma_H^{\alpha_s(M_Z)} = (\pm 0.02 \pm 0.02) \text{ KeV}, \quad (52) \]
\[ \Delta \Gamma_H^{\alpha_s(M_Z)} = (\pm 6.05 \pm 6.02) \text{ KeV}. \quad (53) \]

It shows that the magnitude of \( \Delta \alpha_s(M_Z) \) dominates the error sources. Thus a more precise measurements on the reference point \( \alpha_s(M_Z) \) is important for a more precise pQCD prediction.

By taking the error ranges caused by the UHO-terms that have been predicted via the PAA and B.A. into consideration and by adding all the mentioned errors in quadrature, our final results for the \( H \to gg \) total decay width \( \Gamma_H \) using the PAA predictions are
\[
\begin{align*}
\Gamma_H^{\text{PAA}_{\text{Conv.}}} &= 337.44^{+7.07}_{-6.86} \text{ KeV},
\mu_r^c \in [M_H/2, 2M_H] \quad (54) \\
\Gamma_H^{\text{PAA}_{\text{Conv.}}} &= 337.44^{+10.26}_{-7.51} \text{ KeV}, 
\mu_r^c \in [M_H/4, 4M_H] \quad (55) \\
\Gamma_H^{\text{PAA}_{\text{PMC}_{\infty-s}}} &= 334.45^{+7.07}_{-7.03} \text{ KeV}, \quad (56)
\end{align*}
\]
whose net errors are 4.1%, 5.3% and 4.2%, respectively.

And the final results using the B.A. predictions are
\[
\begin{align*}
\Gamma_H^{\text{B.A.}_{\text{Conv.}}} &= 337.44^{+7.14}_{-6.96} \text{ KeV},
\mu_r^c \in [M_H/2, 2M_H] \quad (57) \\
\Gamma_H^{\text{B.A.}_{\text{Conv.}}} &= 337.44^{+16.98}_{-6.96} \text{ KeV}, 
\mu_r^c \in [M_H/4, 4M_H] \quad (58) \\
\Gamma_H^{\text{B.A.}_{\text{PMC}_{\infty-s}}} &= 334.45^{+6.34}_{-6.29} \text{ KeV}, \quad (59)
\end{align*}
\]
whose net errors are 4.2%, 7.1% and 3.8%, respectively.

IV. SUMMARY

In the paper, we have started from the PMC, together with the use of the iCF property of the renormalizable gauge theories, and proposed a novel single-setting procedure, e.g. the PMC\( \infty-s \)-approach, to eliminate the conventional renormalization scale ambiguities. On the one hand, when enough UHO-terms have been known, the conventional series may achieve small scale-dependent prediction due to the cancellation of scale-dependence among different orders. On the other hand, the PMC\( \infty-s \)-approach removes the scale-dependent terms by using the RGE, and then achieves a scale-invariant prediction at any fixed-order free of conventional renormalization scale ambiguity. By taking the Higgs decays into two gluons as an explicit example, we have shown that the PMC\( \infty-s \)-approach greatly suppresses the residual scale dependence caused by the UHO-terms. To compare with the scale-dependent conventional series, the scale-invariant PMC\( \infty-s \) series provides a more accurate and reliable platform for estimating the UHO-contributions. After applying the PMC\( \infty-s \)-approach, the resultant conformal series also makes its prediction be scheme independent, which satisfies the requirement of the standard renormalization group invariance and can be ensured by the commensurate scale relations among different orders [68, 69].

The MCs approach adopts all the RG-involved non-conformal \( \{\beta_i\} \)-terms to achieve an overall effective coupling of the process, whose argument (the PMC scale) corresponds to the correct momentum flow of the process. While the PMC\( \infty-s \)-approach adopts the property of iCF to fix the overall effective scale, which ensures the scale invariance of the pQCD series at each order by only identifying the \( \{\beta_i\} \)-terms at each order. The scale-setting procedures of the PMC\( \infty-s \)-approach is simpler than the MCs, since it does not need to apply the degeneracy relations. The equivalence of those two single-scale setting approaches indicates that by using the RGE to fix the value of effective coupling is equivalent to require each loop terms satisfy the scale invariance simultaneously, and vice versa. The scale-invariant perturbative series shows the intrinsic perturbative nature of a pQCD observable. Thus the way of using RGE provides a solid way to solve the conventional scale-setting ambiguity. The PMC single-scale setting approach can be applied to any perturbative series in case that we have known the corresponding RGE and correctly applied it to fix the magnitude of the expansion parameter.

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Appendix: The intrinsic conformal coefficients up to N\(^2\)LO-level and coefficients of PMC\( \infty \) scale up to N\(^3\)LL-level

From Eq. (10), the intrinsic conformal coefficients \( L_{i,1c} \) and \( S_i \) can be obtained order-by-order by fixing the the number of flavor \( n_f = 33/2 \):

\[ \mathcal{L}_{1c} = L_1(Q), \quad (60) \]
\[\mathcal{L}_{2,1C} = \mathcal{L}_2(Q)_{|n_f = \frac{31}{2}},\]
\[\mathcal{L}_{3,1C} = \mathcal{L}_3(Q)_{|n_f = \frac{31}{2}} + n \bar{\beta}_1 S_0 \mathcal{L}_1(Q),\]
\[\mathcal{L}_{4,1C} = \mathcal{L}_4(Q)_{|n_f = \frac{31}{2}} + (n + 1) \bar{\beta}_1 S_0 \mathcal{L}_2(Q)_{|n_f = \frac{31}{2}} + n (\bar{\beta}_1 S_1 + \bar{\beta}_2 S_0) \mathcal{L}_1(Q),\]
\[\mathcal{L}_{5,1C} = \mathcal{L}_5(Q)_{|n_f = \frac{31}{2}} + (n + 2) \bar{\beta}_1 S_0 \mathcal{L}_3(Q)_{|n_f = \frac{31}{2}} + (n + 1) \left( \bar{\beta}_1 S_1 + \bar{\beta}_3 S_0 \right) \mathcal{L}_2(Q)_{|n_f = \frac{31}{2}} + n \left( \frac{n + 2}{2} \bar{\beta}_2 S_0^2 + \bar{\beta}_1 S_2 + \bar{\beta}_2 S_1 + \bar{\beta}_3 S_0 \right) \mathcal{L}_1(Q),\]
\[\mathcal{L}_{6,1C} = \mathcal{L}_6(Q)_{|n_f = \frac{31}{2}} + (n + 3) \bar{\beta}_1 S_0 \mathcal{L}_4(Q)_{|n_f = \frac{31}{2}} + (n + 2) \left( \bar{\beta}_1 S_1 + \bar{\beta}_3 S_0 \right) \mathcal{L}_3(Q)_{|n_f = \frac{31}{2}} + (n + 1) \left( \frac{n + 3}{2} \bar{\beta}_1 S_0^2 + \bar{\beta}_1 S_2 + \bar{\beta}_2 S_1 + \bar{\beta}_3 S_0 \right) \mathcal{L}_2(Q),\]
\[S_0 = \frac{1}{n \beta_0 \mathcal{L}_1(Q)} \left[ \mathcal{L}_{2,1C} - \mathcal{L}_2(Q) \right],\]
\[S_1 = \frac{1}{n \beta_0 \mathcal{L}_1(Q)} \left[ \mathcal{L}_{3,1C} - \mathcal{L}_3(Q) - (n + 1) \beta_0 S_0 \mathcal{L}_2(Q) - n \left( \frac{n + 1}{2} \bar{\beta}_2 S_0^2 + \bar{\beta}_1 S_0 \right) \mathcal{L}_1(Q) \right],\]
\[S_2 = \frac{1}{n \beta_0 \mathcal{L}_1(Q)} \left[ \mathcal{L}_{4,1C} - \mathcal{L}_4(Q) - (n + 2) \beta_0 S_0 \mathcal{L}_3(Q) - (n + 1) \left( \frac{n + 2}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_1 S_0 \right) \mathcal{L}_2(Q) - n \left( \frac{n + 1}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_2 S_0 \right) \mathcal{L}_1(Q) \right],\]
\[S_3 = \frac{1}{n \beta_0 \mathcal{L}_1(Q)} \left[ \mathcal{L}_{5,1C} - \mathcal{L}_5(Q) - (n + 3) \beta_0 S_0 \mathcal{L}_4(Q) - (n + 2) \left( \frac{n + 3}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_1 S_0 \right) \mathcal{L}_3(Q) - (n + 1) \left( \frac{n + 2}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_2 S_0 \right) \mathcal{L}_2(Q) - n \left( \frac{n + 1}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_2 S_0 \right) \mathcal{L}_1(Q) \right],\]
\[S_4 = \frac{1}{n \beta_0 \mathcal{L}_1(Q)} \left[ \mathcal{L}_{6,1C} - \mathcal{L}_6(Q) - (n + 4) \beta_0 S_0 \mathcal{L}_5(Q) - (n + 3) \left( \frac{n + 4}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_1 S_0 \right) \mathcal{L}_4(Q) - (n + 2) \left( \frac{n + 3}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_2 S_0 \right) \mathcal{L}_3(Q) - (n + 1) \left( \frac{n + 2}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_2 S_0 \right) \mathcal{L}_2(Q) - n \left( \frac{n + 1}{2} \bar{\beta}_2 S_0^2 + \beta_0 S_1 + \beta_2 S_0 \right) \mathcal{L}_1(Q) \right],\]

where \(\bar{\beta}_i = \beta_i|_{n_f = \frac{33}{2}}\) and \(S_i = S_i|_{n_f = \frac{33}{2}}\). In the above equations \(\mathcal{L}(Q)\) is a short notation for \(\mathcal{L}(Q, Q)\). It is not hard to find that \(S_i\) are 0/0-type limits which always converge to finite values because there are always compo-
nents in the numerator that can always cancel with the \( \beta_0 \) in the denominator.

Then the relations between \( \{ S_i \} \) and \( \{ F_i \} \) can be calculated iteratively as follows:

\[
F_0 = S_0, \quad F_1 = S_1, \quad F_2 = S_2 - \beta_0 \hat{S}_0 S_1, \quad F_3 = S_3 - 2\beta_0 \hat{S}_0 S_2 + \left( \beta_0^2 \hat{S}_0^2 - \beta_1 \hat{S}_0 \right) S_1 - \beta_0 S_1^2,
\]

where \( \hat{S}_0 = S_0 - \ln Q_0^2/Q^2 \).

\[ F_4 = S_4 - 2\beta_0 \hat{S}_0 S_3 - \beta_0^2 \hat{S}_0^2 S_1 - \beta_1^2 S_0^3 S_1 - 3\beta_0^2 \left( \hat{S}_0 S_3^2 + \hat{S}_0^2 S_2 \right) - 3\beta_0 \left( \hat{S}_0 S_3 + S_1 S_2 \right) + \frac{5}{2} \beta_0 \beta_1 \hat{S}_0^2 S_1, \]

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