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Colloquium: The QCD running coupling and the elimination of the scheme-and-scale ambiguities for fixed-order pQCD predictions

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The conventional approach to fixed-order perturbative QCD predictions is based on an arbitrary choice of the renormalization scale, together with an arbitrary range. This *ad hoc* assignment of the renormalization scale causes the coefficients of the QCD running coupling at each order α_s^n to be strongly dependent on the choice of both the renormalization scale and the renormalization scheme. However, such ambiguities are not necessary, since as a basic requirement of renormalization group invariance (RGI), any physical observable must be independent of the choice of both the renormalization scheme and the initial renormalization scale. In fact, if one uses the *Principle of Maximum Conformality* (PMC) to fix the renormalization scale, the coefficients of the pQCD series match the series of conformal theory, and they are thus scheme independent. The PMC predictions also eliminate the divergent *renormalon* contributions which grow strongly as $n!$. The elimination of the scale and scheme ambiguities at all orders relies heavily on how precisely we know the analytic form of the QCD running coupling. Conventional schemes for defining the QCD coupling suffer from a complex and scheme-dependent renormalization group equation (RGE), which is usually solved perturbatively at high orders due to the entanglement of the scheme-running and scale-running behaviors. In this paper, we show that these complications can be avoided by using the newly suggested C-scheme coupling, whose scheme-and-scale running behaviors are governed by the same scheme-independent RGE. As a result, an analytic solution for the running coupling can be achieved at any order. Using the C-scheme coupling, we present a demonstration that the PMC prediction is scheme-independent to all-orders for any renormalization schemes. Given a measurement which sets the magnitude of the coupling at a specific scale such as M_Z, the resulting pQCD predictions, after applying the single-scale PMC, become completely independent of the choice of the renormalization scheme and the initial renormalization scale, thus satisfying all of the conditions of RGI. We illustrate these features for the non-singlet Adler function and for τ decay to $\nu+$ hadrons at four-loop order. The PMC thus systematically eliminates the scheme and scale uncertainties of pQCD predictions, greatly improving the precision of tests of the Standard Model and the sensitivity of collider experiments to new physics.

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Contents

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I. INTRODUCTION

Fixed-order perturbative predictions for observables in Quantum Chromodynamics (QCD) using conventional methods suffer from an uncertainty in fixing the renormalization scale (Brodsky *et al.*, 1983; Grunberg, 1980, 1984; Stevenson, 1981a,b, 1982, 1984). This ambiguity in making fixed-order predictions occurs because one usually assumes an arbitrary renormalization scale, (representing a typical momentum flow of the process) together with an arbitrary range. This *ad hoc* assignment of the renormalization scale causes the coefficients of the QCD running coupling at each order α_s^n to be strongly dependent on the choice of both the renormalization scale and the renormalization scheme.

It is usually assumed that at sufficiently high order, one will eventually achieve reliable predictions and minimal dependence on the guessed renormalization scale for global quantities such as a total cross-section. However, a small scale-dependence for the global quantity could be caused by accidental cancelations among different orders; the scale uncertainty for contributions at each order could still be very large. The running of the QCD-coupling is governed by its *renormalization group equation* (RGE), which is scheme-dependent due to the scheme-dependent $\{\beta_{i\geq 2}\}$-terms. Thus if the $\{\beta_{i\geq 2}\}$-terms have large dependence on the scheme choice, the perturbative predictions based on some schemes could be unreliable; the large expansion coefficients could make the truncation of the perturbative series useless. The resulting uncertainties thus would not be minimized by including more higher-order terms. Even worse, it is known that in general the pQCD series will suffer from divergent *renormalon* contributions which grow as $\alpha_s^n \beta_0^n n!$ (Beneke, 1999; Gardi and Grunberg, 2001). Thus even if a perturbative QCD prediction based on a guessed scale agrees with measurements, one cannot be certain that it is a reliable, accurate representation of the theory.

As a guiding principle, a valid prediction for any physical observable must be independent of the choice of both the initial renormalization scale and the renormalization scheme; this is the central property of *renormalization group invariance* (RGI) (Bogoliubov and Shirkov, 1955; Callan, 1970; Peterman, 1979; Stuckelberg and Peterman, 1953; Symanzik, 1970). Thus a primary goal for testing pQCD reliably is how to set the renormalization scale such that one obtains accurate fixed-order predictions with maximum precision while satisfying the principle of renormalization group invariance. A review of various scale-setting approaches which have been suggested in the literature are summarized in Ref.(Wu *et al.*, 2013).

In contrast to other scale-setting approaches, the *Principle of Maximum Conformality* (PMC) (Brodsky and Wu, 2012; Brodsky and Giustino, 2012; Mojaza *et al.*, 2013; Brodsky *et al.*, 2014; Brodsky and Wu, 2012d,f) determines the value of the renormalization scale of the QCD running coupling α_s based on the properties of RGE and its β-function. When one applies the PMC, all nonconformal β terms are systematically eliminated at each finite order by the choice of the renormalization scale. Since the pQCD series is identical to the series of a conformal theory with $\beta = 0$, the PMC prediction has the essential feature that it is scheme-independent at every finite order. The PMC satisfies the self-consistency conditions of the renormalization group, such as reflectivity, symmetry and transitivity (Brodsky and Wu, 2012c). The resulting PMC predictions thus satisfy all of the basic requirements of RGI. Since the running coupling sums all of the β-terms, the divergent renormalon terms do not appear in the PMC prediction, leading to the convergence of the pQCD series. The PMC provides the underlying principle for the well-known Brodsky-Lepage-Mackenzie (BLM) method (Brodsky *et al.*, 1983). It generalizes the BLM procedure by shifting all $\{\beta_i\}$-terms into the running coupling at all orders, and it reduces to the standard scale-setting procedure of Gell-Mann and Low (GM-L) (Gell-Mann and Low, 1954) in the $N_C \to 0$ QED Abelian limit (Brodsky and Huet, 1998).

The PMC scales are achieved by applying the RGE recursively. The resulting PMC scales reflect the virtuality of the amplitudes relevant to each order. Specific values for the PMC scales are computed as a perturbative expansion, so they have small uncertainties which can vary order-by-order. It has been found that the PMC scales and the resulting fixed-order PMC predictions are to high precision independent of the choice of initial renormalization scale. To make the PMC scale-setting procedures simpler and more easy to be automatized, a single-scale approach (PMC-s), which achieves many of the same PMC goals, has been suggested in Ref.(Shen *et al.*, 2017a). This method effectively

replaces the individual PMC scales at each order by a single scale in the sense of a mean value theorem; moreover, its predictions are explicitly independent of the choice of the initial renormalization scale.

The QCD coupling can be "adiabatically" and continuously evolved not only in scales, but also in the choice of renormalization scheme (Stevenson, 1981a,b, 1982, 1984) by incorporating scheme-running equations, forming the so-called *extended RGEs*. Since along the evolution trajectory of RGEs, no dissimilar scales/schemes are involved, reliable pQCD predictions can be achieved (Lu and Brodsky, 1993). The extended RGEs provide a convenient way for estimating both the scale- and scheme-dependence of pQCD predictions for a physical process. The solution of the scale-running equation can be obtained via an iterative process, which is equivalent to the standard analysis (Chetyrkin, 1997) by using a proper integration constant (Brodsky and Wu, 2012). The scheme-running equations can be solved perturbatively (Lu and Brodsky, 1993).

As we shall show, one can utilize a novel *C-scheme* coupling (Boito *et al.*, 2016) whose scheme-and-scale running behaviors are both governed by a single RGE which is free of scheme-dependent $\{\beta_{i\geq 2}\}$-terms. The value of the parameter C can be chosen to match any conventional renormalization scheme. We shall show that the scheme-independent RGE for the C-scheme coupling leads to scheme-independent pQCD predictions for physical observables, i.e. by using the C-scheme coupling, a strict demonstration on the scheme-independence of PMC prediction to all-orders for any renormalization schemes can be achieved. Thus, by combining the C-scheme coupling with the PMC single-scale approach (PMC-s), the resulting predictions become completely independent of the choice of the renormalization scheme and the initial renormalization scale, satisfying all of the conditions of RGI. This approach thus systematically eliminates the scheme and scale ambiguities of pQCD predictions, greatly improving the precision of tests of the Standard Model and the sensitivity of collider experiments to new physics. Furthermore, since the perturbative coefficients obtained using the PMC-s are identical to those of a conformal theory, one can derive all-orders "commensurate scale relations" (Brodsky *et al.*, 2014; Brodsky and Lu, 1993; Shen *et al.*, 2017b) between physical observables evaluated at specific relative scales. An example is the "Generalized Crewther Relation" (Broadhurst and Kataev, 1993; Brodsky *et al.*, 1996; Crewther, 1997), which shows that the product of $R_{e^+e^-}(s)$ times the integral over the spin-dependent structure functions $g_1(x, Q^2)$ which enters the Bjorken sum rule at a specific value of Q^2/s has no leading-twist radiative QCD corrections at all orders.

The remaining parts of this paper are organized as follows: In Sec.II, we review the RGE and the extended RGE which govern the scheme-and-scale runnings of the QCD coupling. We then define the C-scheme coupling, deduce its scheme-independent RGE, give its analytic solution, and provide the relation between the C-scheme coupling and a conventional coupling. In Sec.III, we present an overview of the PMC, give the formulas for dimensional-regularized $\mathcal{R}_\delta$-schemes and for general C-schemes within the single-scale approach. We then demonstrate the equivalence of PMC, using either the C-scheme coupling or the conventional coupling. By rewriting the pQCD prediction in terms of C-scheme coupling, we will demonstrate how scheme-and-scale independent all-orders predictions can be achieved by applying the PMC single-scale approach. In Sec.IIV, we present numerical results for the two quantities, the non-singlet Adler function and τ decays to $\nu+$ hadrons, up to four-loop level. Sec.V provides a summary.

II. THE RENORMALIZATION SCHEME-AND-SCALE RUNNING OF THE QCD COUPLING

A. The conventional renormalization group equation and its extended version

The definition of the QCD strong coupling $\alpha_s(\mu)$ depends on theoretical conventions such as the choice of the renormalization scheme. Its running behavior in the renormalization scale μ – its RGE – is governed by its logarithmic derivative, the β-function:

$$\mu^2 \frac{\mathrm{d}a_\mu}{\mathrm{d}\mu^2} = \beta(a_\mu) = -a_\mu^2 \sum_{i=0}^{\infty} \beta_i a_\mu^i. \tag{1}$$

For simplicity, we shall set $a_\mu = \alpha_s(\mu)/\pi$, where μ is the renormalization scale, throughout the paper. Various terms in β_0, β_1, $\cdots$, correspond to the one-loop, two-loop, $\cdots$, contributions to the RGE, respectively. The first two terms $\beta_0 = (11 - \frac{2}{3}n_f)/4$ and $\beta_1 = (102 - \frac{38}{3}n_f)/4^2$, where n_f is the number of active quarks, are universal in mass-independent schemes; the remaining $\{\beta_i\}$-terms are scheme-dependent. The explicit form for the $\{\beta_i\}$-terms up to five-loop level in the $\overline{\mathrm{MS}}$-scheme are available in Refs. (Gross and Wilczek, 1973; Politzer, 1973; Caswell, 1974; Tarasov *et al.*, 1980; Larin *et al.*, 1993; Ritbergen *et al.*, 1997; Chetykin, 2005; Czakon, 2005; Baikov *et al.*, 2017).

If one integrates the RGE (1), one obtains

$$\ln \mu_0^2 - \frac{1}{\beta_0 a_{\mu_0}} - \frac{\beta_1}{\beta_0^2} \ln a_{\mu_0} - \int_0^{a_{\mu_0}} \frac{\mathrm{d}a}{\tilde{\beta}(a)} = \ln \mu^2 - \frac{1}{\beta_0 a_\mu} - \frac{\beta_1}{\beta_0^2} \ln a_\mu - \int_0^{a_\mu} \frac{\mathrm{d}a}{\tilde{\beta}(a)}, \tag{2}$$

where μ_0 is a reference scale. We have introduced a new $\tilde{\beta}$-function which is defined as

$$\frac{1}{\tilde{\beta}(a)} \equiv \frac{1}{\beta(a)} + \frac{1}{\beta_0 a^2} - \frac{\beta_1}{\beta_0^2 a}. \tag{3}$$

The advantage of the $\tilde{\beta}$-function lies in the fact that the integral $\int_0^{a_\mu} \mathrm{d}a/\tilde{\beta}(a)$ is free of singularities in the limit $a_\mu \to 0$, so that it can be expressed as a power series in a_μ,

$$\int_0^{a_\mu} \frac{\mathrm{d}a}{\tilde{\beta}(a)} = \left(\frac{\beta_2}{\beta_0^2} - \frac{\beta_1^2}{\beta_0^3}\right) a_\mu + \left(\frac{\beta_3}{2\beta_0^2} - \frac{\beta_2\beta_1}{\beta_0^3} + \frac{\beta_1^3}{2\beta_0^4}\right) a_\mu^2 + \left(\frac{\beta_4}{3\beta_0^2} - \frac{\beta_2^2}{3\beta_0^3} - \frac{2\beta_3\beta_1}{3\beta_0^3} + \frac{\beta_2\beta_1^2}{\beta_0^4} - \frac{\beta_1^4}{3\beta_0^5}\right) a_\mu^3 + \mathcal{O}(a_\mu^4). \tag{4}$$

It is useful to define an *asymptotic scale* Λ by collecting all μ_0-dependent terms on the left-hand-side of Eq.(2) into its definition, leading to the evolution of strong coupling a_μ without reference to a specific choice of μ_0, i.e.

$$\ln \frac{\mu^2}{\Lambda^2} = \frac{1}{\beta_0 a_\mu} + \frac{\beta_1}{\beta_0^2} \ln a_\mu + \int_0^{a_\mu} \frac{\mathrm{d}a}{\tilde{\beta}(a)}. \tag{5}$$

The asymptotic scale Λ is, by definition, scheme dependent. Given a measurement which sets the value of the coupling at a given scale, one can fix Λ for a given scheme by matching the measured value of the coupling to its predicted value as determined by Eq.(5). Notice that this new asymptotic scale Λ differs from the generally adopted asymptotic scale Λ_{QCD} (c.f. the definition given by the PDG (Patrignani *et al.*, 2016)) by an overall parameter; i.e.,

$$\Lambda = \beta_0^{(\beta_1/2\beta_0^2)} \Lambda_{\mathrm{QCD}}. \tag{6}$$

This difference is caused by absorbing different integration constants into the definition of the asymptotic scales. Another example of differing conventions is the 't Hooft scheme ('t Hooft, 1977), where the associated asymptotic scale is $\Lambda'^{tH} = (\beta_0^2/\beta_1)^{2\beta_0^2/\beta_1} \Lambda_{\mathrm{QCD}}$ (Brodsky and Wu, 2012).

It is useful to notice that by using Eq.(5), we can obtain a relation of the couplings at two scales such as μ and Q:

$$\left(\frac{1}{\beta_0 a_\mu} + \frac{\beta_1}{\beta_0^2} \ln a_\mu + \int_0^{a_\mu} \frac{\mathrm{d}a}{\tilde{\beta}(a)}\right) - \left(\frac{1}{\beta_0 a_Q} + \frac{\beta_1}{\beta_0^2} \ln a_Q + \int_0^{a_Q} \frac{\mathrm{d}a}{\tilde{\beta}(a)}\right) = \ln \frac{\mu^2}{Q^2}. \tag{7}$$

If the running coupling is measured at a reference scale Q, then we can fix its value at any other scale without determining the asymptotic scale Λ, thus avoiding any uncertainty coming from the determination of Λ.

Using the relation Eq.(6) and iteratively solving Eq.(5) up to four-loop level yields (Chetyrkin, 1997)

$$\begin{aligned} a_\mu &= \frac{1}{\beta_0 L} - \frac{b_1 \ln L}{(\beta_0 L)^2} + \frac{1}{(\beta_0 L)^3}\left[b_1^2(\ln^2 L - \ln L - 1) + b_2\right] \\ &\quad + \frac{1}{(\beta_0 L)^4}\left[b_1^3\left(-\ln^3 L + \frac{5}{2}\ln^2 L + 2\ln L - \frac{1}{2}\right) - 3b_1 b_2 \ln L + \frac{b_3}{2}\right] + \mathcal{O}\left(\frac{1}{(\beta_0 L)^5}\right), \end{aligned} \tag{8}$$

where $L = \ln(\mu^2/\Lambda_{\mathrm{QCD}}^2)$ and $b_i = \beta_i/\beta_0$.

As a step forward, Stevenson (Stevenson, 1981a,b) has suggested the use of new scheme-running equations which incorporate both the scale and scheme running behaviors in a consistent way. This procedure is called the *extended RGE approach* (Lu and Brodsky, 1993), whose solution has been given in Ref. (Brodsky and Wu, 2012c). As an application, by using the relation of the β-functions between different schemes, i.e. $\beta_{\mathcal{S}}(a_\mu^{\mathcal{S}}) = \beta_{\mathcal{R}}(a_\mu^{\mathcal{R}})\partial a_\mu^{\mathcal{S}}/\partial a_\mu^{\mathcal{R}}$, one can reproduce the Celmaster-Gonsalves relation (Celmaster and Gonsalves, 1978, 1979) for the asymptotic scales of different schemes (Zeng *et al.*, 2016); i.e.

$$\frac{\Lambda^{\mathcal{S}}}{\Lambda^{\mathcal{R}}} = \exp\left(-\frac{f_2}{2\beta_0}\right). \tag{9}$$

Here $\mathcal{S}$ and $\mathcal{R}$ designate two arbitrary renormalization schemes, and the coefficient f_2 is the next-to-leading order term of the coupling $\alpha_\mu^{\mathcal{S}}$ expanded in powers of $\alpha_\mu^{\mathcal{R}}$, i.e. $a_\mu^{\mathcal{R}} = a_\mu^{\mathcal{S}} + f_2(a_\mu^{\mathcal{S}})^2 + f_3(a_\mu^{\mathcal{S}})^3 + \cdots$.

B. A novel scheme-invariant running coupling

Boito and Miravitllas Ref.(Boito *et al.*, 2016) have suggested a novel way to deal with the scheme dependence of QCD couplings based on the Celmaster-Gonsalves relation. They have shown that one can introduce a class of

new couplings $\hat{a}_\mu$, characterized by a single parameter C, whose variation directly compensates for the usual scheme dependence of scale parameter Λ of the corresponding conventional coupling a_μ. In the following, we shall demonstrate that – in distinction to the standard RGE behavior (1) of a_μ, the scale dependence of the resulting C-scheme coupling $\hat{a}_\mu$ is independent of the scheme-dependent $\{\beta_{i\geq 2}\}$-terms, and it is thus explicitly scheme-invariant.

Eq.(5) implies that the conventional a_μ coupling satisfies the following scheme-dependent scale-running behavior

$$\frac{1}{a_\mu} + \frac{\beta_1}{\beta_0}\ln a_\mu = \beta_0\left(\ln\frac{\mu^2}{\Lambda^2} - \int_0^{a_\mu}\frac{\mathrm{d}a}{\tilde{\beta}(a)}\right). \tag{10}$$

As suggested by Ref.(Boito *et al.*, 2016), one can define a new coupling $\hat{a}_\mu = \hat{\alpha}_s(\mu)/\pi$ in the following way:

$$\frac{1}{\hat{a}_\mu} + \frac{\beta_1}{\beta_0}\ln \hat{a}_\mu \;=\; \beta_0\left(\ln\frac{\mu^2}{\Lambda^2} + C\right), \tag{11}$$

where the phenomenological parameter C is introduced which incorporates the effects of all scheme-dependent $\{\beta_{i\geq 2}\}$-terms; i.e. $C = -\int_0^{a_\mu}\mathrm{d}a/\tilde{\beta}(a)$. Different choices of C thus correspond to different renormalization schemes. As will be shown below, there are many advantages in using this single parameter C to characterize the scheme-dependence of the running coupling. By choosing a specific value for $C = C_{\rm RS}$, the running coupling of the C-scheme will become equivalent to the coupling of any conventional renormalization scheme. A subtle point for this equivalence is that the value of C also implicitly depends on the renormalization scale where the C-scheme and the conventional scheme are matched.

By using Eq.(11), the solution of $\hat{a}_\mu$ can be written in terms of the Lambert W-function,

$$\hat{a}_\mu = -\frac{\beta_0}{\beta_1 W_{-1}(z)}, \quad z = -\frac{\beta_0}{\beta_1}\exp\left[-\frac{\beta_0^2}{\beta_1}\left(\ln\frac{\mu^2}{\Lambda^2} + C\right)\right], \tag{12}$$

where $W_{-1}(z)$ is the solution of the equation $W(z)\exp[W(z)] = z$. The function $W(z)$ is a multi-valued function with an infinite number of branches denoted by $W_n(z)$ (Corless *et al.*, 1996). The correct physical branch can be determined by the requirement that $\hat{a}_\mu$ must be real and positive for a real positive scale μ [1]. Since in practice $n_f \leq 6$, we have $z < 0$, and the physical branch is $W_{-1}(z)$. One also finds that $W_{-1}(z)$ monotonically decreases within the region of $z \in (-1/e, 0)$, with $W_{-1}(z) \in (-\infty, -1)$. The ultraviolet limit corresponds to $z \to 0^-$, $W_{-1}(z) \to -\infty$, leading to $\hat{a}_\mu \to 0^+$, as required by asymptotic freedom.

By using Eq.(11), we can obtain a new RGE for the C-scheme coupling $\hat{a}_\mu$ which has a much simpler form than the standard RGE (1):

$$\hat{\beta}(\hat{a}_\mu) = \mu^2\frac{\partial \hat{a}_\mu}{\partial \mu^2} = -\frac{\beta_0\hat{a}_\mu^2}{1-\frac{\beta_1}{\beta_0}\hat{a}_\mu} = -\beta_0\hat{a}_\mu^2\sum_{i=0}^{\infty}(\beta_1/\beta_0)^i\,\hat{a}_\mu^i. \tag{13}$$

At the same time, from Eq.(11), one may also observe that

$$\frac{\partial \hat{a}_\mu}{\partial C} = \hat{\beta}(\hat{a}_\mu). \tag{14}$$

Those two equations indicate that

- The $\hat{\beta}$-function (13) is by definition scheme-independent. Thus the scale-running behavior of the C-scheme coupling $\hat{a}_\mu$ is explicitly scheme-independent since it only depends on the scheme-independent β-coefficients β_0 and β_1. Thus even though the C-scheme coupling $\hat{a}_\mu$ itself is implicitly scheme-dependent, its scale-running behavior can be scheme-independent.

- The scale-running and scheme-running behaviors of $\hat{a}_\mu$ have been explicitly separated – however, each of them separately satisfy the same $\hat{\beta}$-function. As is the case of the conventional RGE (1), the new RGE (13) for the C-scheme coupling can be iteratively solved up to any finite-loop level. It is found that the solution of $\hat{a}_\mu$ up to four-loop level can be obtained from Eq.(8) by replacing

$$a_\mu \to \hat{a}_\mu, \;\; b_i = \beta_i/\beta_0 \to (\beta_1/\beta_0)^i.$$

[1] This conclusion is valid, at least for $\mu^2 \gg \Lambda^2 e^{-C}$.

- Integrating RGE (13) yields a relation of $\hat{a}_\mu$ for any two scales μ_1 and μ_2, i.e.,

$$\frac{1}{\hat{a}_{\mu_2}} = \frac{1}{\hat{a}_{\mu_1}} + \beta_0 \ln \frac{\mu_2^2}{\mu_1^2} - \frac{\beta_1}{\beta_0} \ln \frac{\hat{a}_{\mu_2}}{\hat{a}_{\mu_1}} . \tag{15}$$

  Thus if $\hat{a}$ at the reference scale μ_1 is fixed by a measurement, we can determine its value at any other scale.

- As will be shown below, given the proper choice of C, any coupling constant a_μ which is defined in any conventional scheme can be uniquely expressed by a corresponding C-scheme coupling $\hat{a}_\mu$. For example, in the *effective charge* approach (Grunberg, 1980, 1984), any perturbatively calculable physical observable can be used to define an effective coupling $\hat{a}_\mu$. If the defined effective C-scheme coupling $\hat{a}_\mu$ for an observable is independent of C, Eq.(14) indicates that $\hat{\beta}(\hat{a}_\mu) = 0$, and we will then obtain a scheme-independent pQCD conformal series in $\hat{a}_\mu$ for the corresponding observable.

C. Relation between the C-scheme coupling $\hat{a}_\mu$ and the conventional coupling a_μ

In order to achieve a pQCD prediction using the C-scheme coupling $\hat{a}_\mu$, one needs to obtain a relation between $\hat{a}_\mu$ and the conventional coupling a_μ. We can transform Eq.(11) to the form

$$\frac{1}{\hat{a}_\mu} + \frac{\beta_1}{\beta_0} \ln \hat{a}_\mu = \beta_0\, C + \frac{1}{a_\mu} + \frac{\beta_1}{\beta_0} \ln a_\mu + \beta_0 \int_0^{a_\mu} \frac{\mathrm{d}a}{\tilde{\beta}(a)} ; \tag{16}$$

solving it recursively, we obtain

$$\begin{aligned} a_\mu &= \hat{a}_\mu + C\beta_0 \hat{a}_\mu^2 + \left(\frac{\beta_2}{\beta_0} - \frac{\beta_1^2}{\beta_0^2} + \beta_0^2 C^2 + \beta_1 C \right) \hat{a}_\mu^3 \\ &\quad + \left[\frac{\beta_3}{2\beta_0} - \frac{\beta_1^3}{2\beta_0^3} + \left(3\beta_2 - \frac{2\beta_1^2}{\beta_0} \right) C + \frac{5}{2}\beta_0\beta_1 C^2 + \beta_0^3 C^3 \right] \hat{a}_\mu^4 + \mathcal{O}(\hat{a}_\mu^5), \end{aligned} \tag{17}$$

or inversely,

$$\begin{aligned} \hat{a}_\mu &= a_\mu - C\beta_0 a_\mu^2 + \left(\frac{\beta_1^2}{\beta_0^2} - \frac{\beta_2}{\beta_0} + \beta_0^2 C^2 - \beta_1 C \right) a_\mu^3 \\ &\quad + \left[\frac{\beta_1^3}{2\beta_0^3} - \frac{\beta_3}{2\beta_0} + \left(2\beta_2 - \frac{3\beta_1^2}{\beta_0} \right) C + \frac{5}{2}\beta_0\beta_1 C^2 - \beta_0^3 C^3 \right] a_\mu^4 + \mathcal{O}(a_\mu^5). \end{aligned} \tag{18}$$

This shows that the conventional coupling a_μ at any scale μ can be expanded in terms of the C-scheme coupling $\hat{a}_\mu$ at the same scale, and vice versa.

As an explicit example, consider the conventional coupling a_μ with the $\{\beta_{i\geq 2}\}$-coefficients of the $\overline{\mathrm{MS}}$ renormalization scheme. We then have (Boito *et al.*, 2016),

$$a_\mu^{\overline{\mathrm{MS}}} = \hat{a}_\mu + \frac{9}{4} C \hat{a}_\mu^2 + \left(\frac{3397}{2592} + 4C + \frac{81}{16} C^2 \right) \hat{a}_\mu^3 + \left(\frac{741103}{186624} + \frac{18383}{1152} C + \frac{45}{2} C^2 + \frac{729}{64} C^3 + \frac{445}{144} \zeta(3) \right) \hat{a}_\mu^4 + \cdots \tag{19}$$

where we have set $n_f = 3$, and $\zeta(i)$ is the Riemann ζ-function. Eq.(19) shows that the value of C needs to be introduced as a function of the scale in order to obtain the equivalent C-scheme and $\overline{\mathrm{MS}}$-scheme couplings.

To show explicitly how the C-scheme coupling $\hat{a}$ depends on the parameter C, we present the coupling $\hat{a}$ at the scale M_τ as a function of C in Fig. 1. Here we adopt the world average $\alpha_s^{\overline{\mathrm{MS}}}(M_Z) = 0.1181(11)$ (Patrignani *et al.*, 2016) as the reference value, which runs down to $\alpha_s^{\overline{\mathrm{MS}}}(M_\tau) = 0.3159(95)$ using the four-loop RGE.

- Fig. 1 shows that the coupling $\hat{a}$ monotonously decreases as a function of C. This is confirmed by the fact that the C-scheme $\hat{\beta}(\hat{a}_\mu)$-function (13) is generally negative – the negative $\hat{\beta}(\hat{a}_\mu)$-function implies that the coupling must monotonically decrease with the increment of C.

- By choosing a suitable C, the new coupling $\hat{a}_\mu$ becomes equivalent to the coupling a_μ defined for any corresponding conventional scheme; i.e. $a_\mu = \hat{a}_\mu|_C$. At a different scale μ, a different C needs to be introduced in order to ensure the equivalence of the couplings at the same scale. For example, we have

$$a_{M_\tau}^{\overline{\mathrm{MS}}} = \hat{a}_{M_\tau}(C = -0.0818) \;\text{ and }\; a_{M_Z}^{\overline{\mathrm{MS}}} = \hat{a}_{M_Z}(C = 0.7285).$$

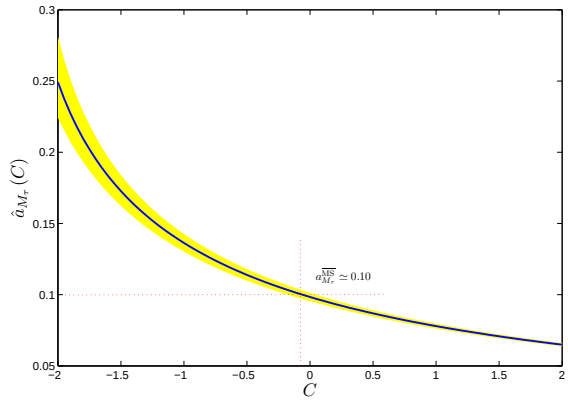

FIG. 1 The C-scheme coupling $\hat{a}_{M_\tau}$ as a function of C at the scale M_τ, which is calculated by using the relation (16) up to four-loop level. We adopt $\alpha_s^{\overline{\rm MS}}(M_\tau) = 0.3159(95)$ as the reference value. The solid line represents the center value, and the shaded band corresponds to the uncertainty $\Delta\alpha_s(M_\tau) = \pm 0.0095$. The crossing point of the two dotted lines indicates $\hat{a}_{M_\tau}(C = -0.0818) = a_{M_\tau}^{\overline{\rm MS}}$.

III. SCHEME-AND-SCALE INDEPENDENT PQCD PREDICTIONS USING PMC SCALE-SETTING

The pQCD approximant of an observable up to $n_{\rm th}$-order level can be generally expressed as

$$\rho_n(Q) = \sum_{i=1}^{n} r_i(\mu/Q) a_\mu^{i+p} \tag{20}$$

or

$$\rho_n(Q) = \sum_{i=1}^{n} \hat{c}_i(\mu/Q) \hat{a}_\mu^{i+p}, \tag{21}$$

where μ is the renormalization scale and Q is the kinematic scale of the process at which it is measured. Without losing generality, we can set the power of the coupling associated with the tree-level term as 1, or equivalently $p = 0$. The parameters r_i and $\hat{c}_i$ are the perturbative coefficients for the conventional coupling a_μ and the corresponding C-scheme coupling $\hat{a}_\mu$. Their relations can be obtained by using the relation (17) between the C-scheme coupling $\hat{a}_\mu$ and the conventional coupling a_μ,

$$\hat{c}_1 = r_1, \tag{22}$$

$$\hat{c}_2 = r_2 + \beta_0 r_1 C, \tag{23}$$

$$\hat{c}_3 = r_3 + (\beta_1 r_1 + 2\beta_0 r_2) C + \beta_0^2 r_1 C^2 + r_1 \left(\frac{\beta_2}{\beta_0} - \frac{\beta_1^2}{\beta_0^2}\right), \tag{24}$$

$$\hat{c}_4 = r_4 + \left(3\beta_0 r_3 + 2\beta_1 r_2 + 3\beta_2 r_1 - \frac{2\beta_1^2 r_1}{\beta_0}\right) C + \left(3\beta_0^2 r_2 + \frac{5}{2}\beta_1\beta_0 r_1\right) C^2 + r_1 \beta_0^3 C^3 + r_1\left(\frac{\beta_3}{2\beta_0} - \frac{\beta_1^3}{2\beta_0^3}\right) + r_2\left(\frac{2\beta_2}{\beta_0} - \frac{2\beta_1^2}{\beta_0^2}\right), \tag{25}$$

$$\cdots$$

The authors of Refs.(Boito *et al.*, 2016; Jamin and Miravitllas, 2016) have investigated the possibility of obtaining an "optimized" prediction for the truncated pQCD series using the C-scheme coupling by exploiting its scheme dependence. In their treatment, by fixing $\mu \equiv Q$ and varying C within a possible domain, an optimal C-value, and thus an optimal scheme, is determined by requiring the absolute value of the last known term $\hat{c}_n(Q/Q)\hat{a}_Q^n$ to be at its minimum. However,

- We note that the idea of requiring the magnitude of the last known term of the pQCD series to be at its minimum is similar to the postulate of the *Principle of Minimum Sensitivity* (PMS) (Stevenson, 1981a,b, 1982,

1984), in which the optimal scheme is determined by directly requiring all unknown higher-order terms to vanish. Thus this application of optimization to the C-scheme coupling approach meets the same problems of PMS, cf. Refs.(Ma *et al.*, 2015; Wu *et al.*, 2015): It does not satisfy the self-consistency conditions of the renormalization group, such as reflectivity, symmetry and transitivity (Brodsky and Wu, 2012c); Its pQCD convergence is accidental and questionable; it disagrees with Gell Mann-Low scale setting when applied to QED cases; and it gives unphysical results for jet production in e^+e^- annihilation; etc..

- The optimal value of C is different for a different fixed-order prediction, which need to be redetermined when new perturbative terms are known. Although this approach of using the C-scheme coupling could be considered as a practical way to improve pQCD precision, similar to the PMS approach, it cannot be considered as the solution to the conventional scheme-and-scale setting ambiguities.

In contrast to the PMS, the PMC identifies all the RG-involved scheme-dependent $\{\beta_i\}$-terms in the perturbative series and eliminate them by shifting the scales of the running coupling. After applying the PMC, the coefficients ρ_n of α_s^n match the corresponding conformal series, and thus the prediction is scheme independent in general. We have presented in Ref. (Mojaza *et al.*, 2013; Brodsky *et al.*, 2014) an explicit demonstration that PMC scale-setting leads to scheme-independent pQCD predictions for any dimensional-like enormalization scheme, with the generalized subtraction $-\ln 4\pi+\gamma_E+\delta$, which we label as the $\mathcal{R}_\delta$-scheme. Thus different values of δ indicate different dimensional-like scheme; e.g. $\delta = 0$ is the $\overline{\rm MS}$-scheme, and $\delta = \ln 4\pi - \gamma_E$ is the unsubtracted MS-scheme. More explicitly if the perturbative coefficient ρ_n has been calculated using the R_δ-scheme, they satisfy

$$\frac{\partial \rho_n}{\partial \delta} = -\beta(a_\mu)\frac{\partial \rho_n}{\partial a_\mu}. \tag{26}$$

Thus after eliminating all of the $\{\beta_i\}$-terms by applying the PMC, one obtains $\partial\rho_n|_{\rm PMC}/\partial\delta = 0$, proving that the PMC prediction $\rho_n|_{\rm PMC}$ is independent of the value of δ and thus any choice of the dimensionally regulated $\mathcal{R}_\delta$-schemes.

We will now generalize this procedure to see whether one can eliminate all scheme-dependent C-terms in a pQCD approximant by applying the PMC. Since the parameter C identifies any choice of the renormalization scheme, we will then achieve a general demonstration of the scheme-independence of the PMC pQCD predictions for any renormalization scheme.

A. An overview of the PMC scale-setting

A rigorous demonstration of the scheme-independence of PMC predictions for any dimensional-like $\mathcal{R}_\delta$-scheme has been given in Refs.(Mojaza *et al.*, 2013; Brodsky *et al.*, 2014). The PMC provides a systematic way to set the optimized renormalization scale up to all order. The PMC procedure follows these steps

- First, we perform a pQCD calculation of an observable, taking any renormalization scheme at an arbitrary initial renormalization scale. The initial renormalization scale only need to be large enough to ensure the reliability of the perturbative prediction. For example, one may choose the renormalization scheme to be the usually adopted $\overline{\rm MS}$-scheme; after applying the PMC, the final pQCD prediction will be shown it to be independent of this choice, since the PMC is consistent with RGI.

- Second, we identify the β terms in the pQCD series. This can be achieved with the help of the degeneracy relations among different orders which identify which terms in the pQCD series are associated with the RGE and which terms are not. Alternatively, one can use the δ dependence of the series to identify the β terms. One can also rearrange all the perturbative coefficients, which are usually expressed as an n_f-power series, into $\{\beta_i\}$-terms or non-$\{\beta_i\}$-terms. One needs to be careful using this method to ensure that the UV-free light-quark loops are not related to the $\{\beta_i\}$-terms; they should be identified as non-conformal ones and should be kept unchanged when doing the $n_f \to \{\beta_i\}$ transformation. In practice, one can also apply PMC scale setting by directly dealing with the n_f-power series without transforming them into the $\{\beta_i\}$-terms (Brodsky and Wu, 2012). If the n_f-terms are treated correctly, the results for these treatments are equivalent since they lead to the same resummed "conformal" series up to all orders. Any scale difference between the two approaches at each order is comparatively small; it is systematically reduced as more $\{\beta_i\}$-terms are taken into account (Bi *et al.*, 2015).

- Third, we absorb different types of $\{\beta_i\}$-terms into the strong coupling in an order-by-order manner. Different types of $\{\beta_i\}$-terms as determined from the RGE lead to different running behaviors of the strong coupling at different orders, and hence, determine distinct PMC scales at each order. The PMC scales themselves are given by a perturbative expansion series in the strong coupling.

- Finally, through these steps, all non-conformal $\{\beta_i\}$-terms are resummed into the running coupling such that the remaining terms in the perturbative series are identical to those of the corresponding conformal theory, thus leading to a scheme-independent prediction. The scheme-independence of the PMC prediction is a general result; it has been explicitly demonstrated for dimensional-like R_δ-scheme. Since a different renormalization scale generally appears at each order, we call this approach as the PMC multi-scale approach.

Recently, we have suggested a novel single-scale PMC approach, labeled as PMC-s, which sets a single overall PMC scale for the pQCD approximant (Shen *et al.*, 2017a). This PMC-s scale effectively replaces the individual PMC scales at each order in the sense of a mean-value theorem. The single-scale approach avoids the problem of very small arguments of the running coupling appearing at any specific order; e.g., when a soft gluon carries the momentum flow. Some examples appear in the analysis of the Bjorken sum rule (Deur *et al.*, 2017), the analysis of hadronic τ decay ,and the static quark potential (Brodsky *et al.*, 2014).

The single-scale approach makes the implementation and automation of PMC scale-setting simpler and more transparent. It is, however, effectively equivalent to the multi-scale approach (Shen *et al.*, 2017a). The PMC-s fixes the renormalization scale by directly requiring all the known RG-dependent nonconformal terms to vanish. The effective PMC scale have been observed in two examples to approach a steady point with increasing loop order. Moreover, the difference between the two nearby values decreases as more high-order loop-terms are included. The rapid pQCD convergence of the effective PMC scale indicates that the single PMC scale converges rapidly as more loop corrections are included.

The single-scale PMC-s approach can be adopted as a reliable substitution for the multi-scale approach for setting the scale for high-energy processes, particularly when one does not need detailed information at each order.

In summary, the PMC-s inherits most of the features of the multi-scale approach: its predictions are also scheme independent due to the resulting conformal series, and the convergence of the pQCD expansion is also greatly improved due to the elimination of the divergent renormalon terms. On the other hand, in some leading-twist processes such as single-spin asymmetries in deep inelastic scattering (Brodsky *et al.*, 2002) or the double Boer-Mulders effect in lepton pair production (Brodsky *et al.*, 2003), the scale of the running coupling at specific orders will be physically soft since these processes involve gluonic initial-state or final-state interactions at relatively small momentum transfer. Thus in this case the PMC multi-scale approach is required.

B. The PMC scale-setting for dimensional-like $\mathcal{R}_\delta$-scheme

The $\mathcal{R}_\delta$-scheme introduces a generalization of the conventional dimensional regularization schemes, where a constant $-\delta$ is subtracted in addition to the standard subtraction $\ln 4\pi - \gamma_E$ of the $\overline{\rm MS}$-scheme. The $\mathcal{R}_\delta$-scheme provides a natural explanation of the degeneracy relations which are general properties of the non-Abelian gauge theory and underly the resulting conformal features of the pQCD series (Bi *et al.*, 2015). By using the general displacement relation for the running coupling at any two scales, one can obtain the general pattern of the $\{\beta_i\}$-terms at each order, which naturally implies the wanted degeneracy relations among different terms; e.g., the coefficients for $\beta_0 a_\mu^2$, $\beta_1 a_\mu^3$, $\cdots$, $\beta_i a_\mu^{i+2}$ are the same.

The pQCD approximants among different $\mathcal{R}_\delta$-schemes are simply related by a scale shift. We can derive general pQCD expression in the $\mathcal{R}_\delta$-schemes by using the displacement relation between couplings at different scales,

$$a_\mu = a_{\mu_\delta} + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{{\rm d}^n a_\mu}{({\rm d}\ln\mu^2)^n}\bigg|_{\mu=\mu_\delta} (-\delta)^n, \tag{27}$$

where $\delta = \ln \mu_\delta^2/\mu^2$. Thus one can rewrite the pQCD prediction (20) as (Mojaza *et al.*, 2013; Brodsky *et al.*, 2014)

$$\begin{aligned}\rho_n(Q) \;=\; & r_1 a_{\mu_\delta} + (r_2 + \beta_0 r_1 \delta) a_{\mu_\delta}^2 + [r_3 + \beta_1 r_1 \delta + 2\beta_0 r_2 \delta + \beta_0^2 r_1 \delta^2] a_{\mu_\delta}^3 \\ & + [r_4 + \beta_2 r_1 \delta + 2\beta_1 r_2 \delta + 3\beta_0 r_3 \delta + 3\beta_0^2 r_2 \delta^2 + \beta_0^3 r_1 \delta^3 + \frac{5}{2}\beta_1\beta_0 r_1 \delta^2] a_{\mu_\delta}^4 + \mathcal{O}(a_{\mu_\delta}^5).\end{aligned} \tag{28}$$

It is easy to confirm that,

$$\frac{\partial \rho_n}{\partial \delta} = -\frac{\partial a_{\mu_\delta}}{\partial \delta}\frac{\partial \rho_n}{\partial a_{\mu_\delta}} = -\mu_\delta^2 \frac{\partial a_{\mu_n}}{\partial \mu_\delta^2}\frac{\partial \rho_n}{\partial a_{\mu_\delta}} = -\beta(a_{\mu_\delta})\frac{\partial \rho_n}{\partial a_{\mu_\delta}}. \tag{29}$$

This shows that when the non-conformal terms associated with the $\beta(a_{\mu_\delta})$-function have been removed, one can achieve a scheme-independent prediction; i.e. $\beta(a_{\mu_\delta}) \to 0$ indicates $\partial\rho_n/\partial\delta \to 0$. The PMC scales determined by the

non-conformal terms depend on the choice of renormalization scheme, which however are compensated by scheme-dependent coefficients $r_{i,0}$, leading to the final conformal and scheme-independent pQCD series. This is also consistent with the commensurate scale relations (Brodsky and Lu, 1993; Shen *et al.*, 2017b) among different orders.

By explicitly showing the β-pattern at each perturbative order; i.e., by replacing the coefficients r_i with $r_{i,j}$, the pQCD prediction ρ_n as defined in Eq.(20) can be rewritten in the following form

$$\begin{aligned}\rho_n(Q) &= \sum_{i=1}^{n} r_i(\mu/Q)a_\mu^i \\ &= r_{1,0}a_\mu + [r_{2,0}+\beta_0 r_{2,1}]\,a_\mu^2 + \left[r_{3,0}+\beta_1 r_{2,1}+2\beta_0 r_{3,1}+\beta_0^2 r_{3,2}\right]a_\mu^3 \\ &\quad + \left[r_{4,0}+\beta_2 r_{2,1}+2\beta_1 r_{3,1}+\frac{5}{2}\beta_1\beta_0 r_{3,2}+3\beta_0 r_{4,1}+3\beta_0^2 r_{4,2}+\beta_0^3 r_{4,3}\right]a_\mu^4+\cdots. \end{aligned} \tag{30}$$

The non-conformal coefficients $r_{i,j(\geq 1)}$ are general functions of μ and Q, which are usually in form of $\ln\mu/Q$. For convenience, we identify the coefficients $r_{i,j(\geq 1)}$ as $r_{i,j}=\sum_{k=0}^{j} C_j^k \ln^k(\mu^2/Q^2)\hat{r}_{i-k,j-k}$, in which $\hat{r}_{i,j}=r_{i,j}|_{\mu=Q}$ and the combination coefficient $C_j^k = j!/k!(j-k)!$. The conformal coefficients are free from μ-dependence, e.g., $r_{i,0}\equiv\hat{r}_{i,0}$.

Next, we rewrite the pQCD expansion (30) into a compact form as

$$\rho_n(Q)=\sum_{i\geq 1}^{n} r_{i,0}a_\mu^i + \sum_{i\geq 1, j\geq 1}^{i+j\leq n}(-1)^j\left[i\beta(a_\mu)a_\mu^{i-1}\right]r_{i+j,j}\Delta_i^{(j-1)}(a_\mu). \tag{31}$$

For a fourth-order prediction, we need to know the first three $\Delta_i^{(j-1)}(x)$, which are

$$\Delta_i^{(0)}(x) = 1, \tag{32}$$

$$\Delta_i^{(1)}(x) = \frac{1}{2!}\left[\frac{\partial\beta(x)}{\partial x}+(i-1)\frac{\beta(x)}{x}\right], \tag{33}$$

$$\Delta_i^{(2)}(x) = \frac{1}{3!}\left[\beta(x)\frac{\partial^2\beta(x)}{(\partial x)^2}+\left(\frac{\partial\beta(x)}{\partial x}\right)^2+3(i-1)\frac{\beta(x)}{x}\frac{\partial\beta(x)}{\partial x}+(i-1)(i-2)\frac{\beta(x)^2}{x^2}\right]. \tag{34}$$

In the second summation of Eq.(31), we need to keep the expansion up to a_μ^n-order.

Following the standard PMC procedures, we are ready to fix the PMC scale and obtain the required PMC predictions.

For the multi-scale PMC approach, we obtain the following conformal series for a pQCD approximant up to $n_{\rm th}$-order level,

$$\rho_n(Q)|_{\rm PMC}=\sum_{i=1}^{n} r_{i,0}a_{Q_i}^i, \tag{35}$$

where only the conformal coefficients $r_{i,0}$ remain, and the PMC scales Q_i for each order are determined by recursively absorbing the $\{\beta_i\}$-terms into the coupling at the corresponding order, which satisfy

$$\sum_{j\geq 0}\Delta_i^{(j)}(a_\mu)\ln^{j+1}\frac{Q_i^2}{\mu^2}=\sum_{j\geq 0}(-1)^{j+1}\Delta_i^{(j)}(a_\mu)\frac{r_{i+j+1,j+1}}{r_{i,0}}, \tag{36}$$

which leads to

$$\ln\frac{Q_i^2}{Q^2} = \sum_{0\leq j\leq(n-1-i)} P_{i,j}a_\mu^j. \quad i\in[1,(n-1)]. \tag{37}$$

For a $n_{\rm th}$-order prediction, we can fix $(n-1)$ PMC scales. The above expressions show that the PMC scale Q_i is given as a perturbative series; any residual scale dependence in Q_i is due to unknown high-order terms. This is the first kind of residual scale dependence. However, we have no information on how to set the scale for the highest-order running coupling; in practice, it can be set as the finally determined PMC scale, i.e. $Q_n=Q_{n-1}$. This treatment leads to the second kind of residual scale dependence. In practice, we have found that those two residual scale dependence, in comparison with the conventional scale dependence, are quite small even at low orders. This is due to a much

faster pQCD convergence after applying the PMC (the first kind also suffers from exponential suppression). Solving Eq.(36) iteratively, we can get the perturbative coefficients $P_{i,j}$ for the PMC scales. For example, for a fourth-order prediction, we have

$$P_{i,0} = -\frac{\hat{r}_{i+1,1}}{r_{i,0}}, \tag{38}$$

$$P_{i,1} = \frac{(i+1)(r_{i+1,1}^2 - r_{i,0}r_{i+2,2})}{2r_{i,0}^2}\beta_0, \tag{39}$$

$$P_{i,2} = \frac{(i+2)(r_{i+1,1}^2 - r_{i,0}r_{i+2,2})}{2r_{i,0}^2}\beta_1 - \frac{(i+1)[(2i+1)r_{i+1,1}^3 - 3(i+1)r_{i,0}r_{i+1,1}r_{i+2,2} + (i+2)r_{i,0}^2 r_{i+3,3}]}{6r_{i,0}^3}\beta_0^2. \tag{40}$$

For the single-scale approach (PMC-s), the resulting conformal series up to $n_{\rm th}$-order level changes to

$$\rho_n(Q)|_{\rm PMC-s} = \sum_{i\geq 1}^{n} r_{i,0} a_{Q_\star}^i, \tag{41}$$

where a single effective PMC scale $Q_\star$ is introduced, which is determined by requiring all the non-conformal terms to vanish simultaneously, i.e.

$$\sum_{i\geq 1, j\geq 1, 0\leq k\leq j} (-1)^j \ln^k \frac{Q_\star^2}{Q^2}\left[i\beta(a_{Q_\star})a_{Q_\star}^{i-1}\right] C_j^k \Delta_i^{(j-1)}(a_{Q_\star})\hat{r}_{i+j-k,j-k} = 0\ , \tag{42}$$

which leads to

$$\ln\frac{Q_\star^2}{Q^2} = \sum_{i=0}^{n-2} S_i a_{Q_\star}^i. \tag{43}$$

Solving Eq.(42) iteratively, we can get the perturbative coefficients S_i. For example, for a fourth-order prediction, we have

$$S_0 = -\frac{\hat{r}_{2,1}}{\hat{r}_{1,0}}, \tag{44}$$

$$S_1 = \frac{2\left(\hat{r}_{2,0}\hat{r}_{2,1} - \hat{r}_{1,0}\hat{r}_{3,1}\right)}{\hat{r}_{1,0}^2} + \frac{\hat{r}_{2,1}^2 - \hat{r}_{1,0}\hat{r}_{3,2}}{\hat{r}_{1,0}^2}\beta_0, \tag{45}$$

$$S_2 = \frac{3\hat{r}_{1,0}\left(\hat{r}_{3,0}\hat{r}_{2,1} - \hat{r}_{1,0}\hat{r}_{4,1}\right) + 4\hat{r}_{2,0}\left(\hat{r}_{1,0}\hat{r}_{3,1} - \hat{r}_{2,0}\hat{r}_{2,1}\right)}{\hat{r}_{1,0}^3} + \frac{3\hat{r}_{1,0}\hat{r}_{2,1}\hat{r}_{3,2} - \hat{r}_{1,0}^2\hat{r}_{4,3} - 2\hat{r}_{2,1}^3}{\hat{r}_{1,0}^3}\beta_0^2$$
$$+\frac{3\left(\hat{r}_{2,1}^2 - \hat{r}_{1,0}\hat{r}_{3,2}\right)}{2\hat{r}_{1,0}^2}\beta_1 + \frac{3\hat{r}_{1,0}\left(2\hat{r}_{2,1}\hat{r}_{3,1} - \hat{r}_{1,0}\hat{r}_{4,2}\right) + \hat{r}_{2,0}\left(2\hat{r}_{1,0}\hat{r}_{3,2} - 5\hat{r}_{2,1}^2\right)}{\hat{r}_{1,0}^3}\beta_0. \tag{46}$$

As shown in Eqs.(44, 45, 46), there are some identical combinations in the scale expansion series among different orders, which are consistent with the degeneracy relations among different orders; e.g., the coefficients of $(i+2)\beta_i a^{i+1}(Q)$ are the same. These equations show that the scale $Q_\star$ has no relation to the initial scale μ at any fixed order. Thus the PMC-s has only the first kind of residual scale dependence, whose magnitude is also smaller than the case of the multi-scale approach, since the precision of the PMC scales at various orders are generally different due to their $\{\beta_i\}$-terms are known at different orders. Moreover, the pQCD series for the observable converges rapidly; thus any residual scale dependence due to uncalculated high-order terms will be greatly suppressed. For example, the conventional approach assigns an uncertainty of $\left(^{+1.0\%}_{-3.0\%}\right)$, $\left(^{+0.3\%}_{-1.6\%}\right)$ or $\left(^{+0.4\%}_{-0.2\%}\right)$ to the two-loop, three-loop, and the four-loop approximants of the ratio $R_{e^+e^-}(Q = 31.6\text{GeV})$ by assuming the range $\mu \in [1/2Q, 2Q]$, respectively; as a comparison, the single-scale PMC prediction on $R_{e^+e^-}(Q = 31.6\text{GeV})$ is unchanged within the same choices of μ (Shen *et al.*, 2017a). Thus, the PMC single-scale approach PMC-s could be adopted as a valid substitution for the PMC multi-scale approach for setting the renormalization scale for high-energy processes, particularly when one does not need detailed information at each order.

C. The PMC scale-setting for a general C-scheme

By using the relation (17) between the C-scheme coupling $\hat{a}_\mu$ and the conventional coupling a_μ, we transform the pQCD approximant $\rho_n(Q)$ as

$$\hat{\rho}_n(Q) = \sum_{i=1}^{n} \hat{c}_i(\mu/Q)\hat{a}_\mu^i. \tag{47}$$

Here we are considering at least the next-to-leading order pQCD correction to the pQCD prediction; i.e. $n \geq 2$. The coefficients $\hat{c}_i$ can be related to the coefficients $r_{i,j}$ for conventional running coupling from Eqs.(22, 23, 24, 25, 30). We shall adopt the same notation $\hat{r}_{i,j} = r_{i,j}|_{\mu=Q}$ for our following treatment, in which the conformal coefficient $r_{i,0} = \hat{r}_{i,0}$. These equations show the non-conformal part of the coefficients $\hat{c}_i$ have a more complex $\{\beta_i\}$-structure; it can be schematically written as

$$\hat{c}_i(\mu/Q) = \hat{r}_{i,0} + g_i\left(\mu/Q, \{\beta_j^m\}\right) + h_i\left(\mu/Q, \{\beta_k^l/\beta_0^n\}\right), \tag{48}$$

where $j \geq 0$, $l, m, n, k \geq 1$, the functions g_i and h_i can be read from the known coefficients $\hat{c}_i$. Due to this complex $\{\beta_i\}$-structure, it is difficult to distribute g_i and h_i into running couplings at different orders, although this is important for determining the correct running coupling at each perturbative order. To avoid this problem, we will treat $(g_i + h_i)$ together and adopt the single-scale PMC approach to eliminate all the RG-involved $\{\beta_i\}$-terms [2].

By using Eq.(47), we obtain

$$\frac{\partial \hat{\rho}_n}{\partial C} = -\frac{\partial \hat{a}_\mu}{\partial C}\frac{\partial \hat{\rho}_n}{\partial \hat{a}_\mu} = -\mu^2\frac{\partial \hat{a}_\mu}{\partial \mu^2}\frac{\partial \hat{\rho}_n}{\partial \hat{a}_\mu} = -\hat{\beta}(\hat{a}_\mu)\frac{\partial \hat{\rho}_n}{\partial \hat{a}_\mu}, \tag{49}$$

where we have used the fact that the scale-running and scheme-running of $\hat{a}_\mu$ satisfy the same $\hat{\beta}$-function. Eq.(49) shows that when the non-conformal terms associated with the $\hat{\beta}(\hat{a}_\mu)$-function have been removed, one can achieve a scheme-independent prediction at any fixed order, i.e. $\hat{\beta}(\hat{a}_\mu) \to 0$ indicates $\partial\hat{\rho}_n/\partial C \to 0$. Eq.(49) agrees with the conclusion of Eq.(29) which is derived using the $\mathcal{R}_\delta$-scheme. The present conclusion however is much more general, since the value of C is arbitrary and could be referred to as any renormalization scheme.

Following the single-scale PMC procedures, an effective scale $Q_\star$ is introduced to eliminate all nonconformal terms. The scale $Q_\star$ is thus determined by requiring

$$\sum_{i=1}^{n}\left[g_i\left(Q_\star/Q, \{\beta_j^m\}\right) + h_i\left(Q_\star/Q, \left\{\beta_{k(\geq 1)}^l/\beta_0^{n(\geq 1)}\right\}\right)\right]\hat{a}_{Q_\star}^i = 0. \tag{50}$$

This equation can be solved recursively, and we can express the solution as a power series in $\hat{a}_{Q_\star}$, i.e.,

$$\ln\frac{Q_\star^2}{Q^2} = \sum_{i=0}^{n-2}\hat{S}_i\hat{a}_{Q_\star}^i, \tag{51}$$

whose first three coefficients are

$$\hat{S}_0 = -\frac{\hat{r}_{2,1}}{\hat{r}_{1,0}} - C, \tag{52}$$

$$\hat{S}_1 = \frac{2\left(\hat{r}_{2,0}\hat{r}_{2,1} - \hat{r}_{1,0}\hat{r}_{3,1}\right)}{\hat{r}_{1,0}^2} + \frac{\hat{r}_{2,1}^2 - \hat{r}_{1,0}\hat{r}_{3,2}}{\hat{r}_{1,0}^2}\beta_0 + \frac{\beta_1^2}{\beta_0^3} - \frac{\beta_2}{\beta_0^2}, \tag{53}$$

$$\begin{aligned}\hat{S}_2 = {} & \frac{3\hat{r}_{1,0}\left(\hat{r}_{3,0}\hat{r}_{2,1} - \hat{r}_{1,0}\hat{r}_{4,1}\right) + 4\hat{r}_{2,0}\left(\hat{r}_{1,0}\hat{r}_{3,1} - \hat{r}_{2,0}\hat{r}_{2,1}\right)}{\hat{r}_{1,0}^3} + \frac{3\hat{r}_{1,0}\hat{r}_{2,1}\hat{r}_{3,2} - \hat{r}_{1,0}^2\hat{r}_{4,3} - 2\hat{r}_{2,1}^3}{\hat{r}_{1,0}^3}\beta_0^2 \\ & + \frac{3\left(\hat{r}_{2,1}^2 - \hat{r}_{1,0}\hat{r}_{3,2}\right)}{2\hat{r}_{1,0}^2}\beta_1 + \frac{3\hat{r}_{1,0}\left(2\hat{r}_{2,1}\hat{r}_{3,1} - \hat{r}_{1,0}\hat{r}_{4,2}\right) + \hat{r}_{2,0}\left(2\hat{r}_{1,0}\hat{r}_{3,2} - 5\hat{r}_{2,1}^2\right)}{\hat{r}_{1,0}^3}\beta_0 - \frac{\beta_1^3}{2\beta_0^4} + \frac{\beta_2\beta_1}{\beta_0^3} - \frac{\beta_3}{2\beta_0^2}.\end{aligned} \tag{54}$$

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[2] As a comparison, the non-conformal coefficients $r_{i,j(\geq 1)}$ for conventional running coupling, as shown by Eq.(30), are superposition of RGEs for each running coupling, thus they can be conveniently adopted for determining the correct PMC scale at each perturbative order.

It is interesting to find that all high-order coefficients $\hat{S}_i$ $(i \geq 1)$ are free of the scheme parameter C. By using the definition of C-scheme coupling (11), we obtain

$$\begin{aligned} \frac{1}{\hat{a}_{Q_\star}} + \frac{\beta_1}{\beta_0} \ln \hat{a}_{Q_\star} &= \beta_0 \left(\ln \frac{Q_\star^2}{\Lambda^2} + C \right) \\ &= \beta_0 \left(\ln \frac{Q^2}{\Lambda^2} - \frac{\hat{r}_{2,1}}{\hat{r}_{1,0}} + \sum_{i\geq 1}^{n-2} \hat{S}_i \hat{a}_{Q_\star}^i \right). \end{aligned} \tag{55}$$

The second equation shows that, even though the effective scale $Q_\star$ depends on the choice of C, the coupling $\hat{\alpha}_{Q_\star}$ is independent of the choice of C at any fixed order.

Thus, after fixing the scale $Q_\star$, we achieve a C-scheme independent pQCD series

$$\hat{\rho}_n(Q)|_{\rm PMC} = \sum_{i\geq 1}^{n} r_{i,0} \hat{a}_{Q_\star}^i. \tag{56}$$

The pQCD series depends on the initial choice of scheme via the coefficients $r_{i,j}$ and the $\{\beta_{i\geq 2}\}$-functions. Thus, Eq.(56) indicates the scheme-independence of the C-scheme predictions is equivalent to the scheme-independence of the initial choice of scheme, and vice versa. The demonstration of C-scheme independence, as shown by Eq.(49), shows the pQCD predictions are scheme independent for any choice of the initial scheme.

Given a measurement of the running coupling at a reference scale Q, a_Q, one can determine the value of Λ for a specific scheme by using its $\{\beta_i\}$-functions. By using the above formulas, we obtain pQCD predictions independent of any choice of scheme (represented by any choice of C). This demonstrates to any orders the scheme-independent of the PMC predictions – Given one measurement which sets the value of the coupling at a scale, the resulting PMC predictions are independent of the choice of renormalization scheme.

D. Equivalence of the PMC predictions for $\mathcal{R}_\delta$-schemes for conventional and C-scheme couplings

In the case of the dimensional-like $\mathcal{R}_\delta$-renormalization schemes, the PMC predictions for the conventional coupling (Eq.(41)) and the C-scheme coupling (Eq.(56)) are exactly the same. This equivalence is due to the fact that

- By eliminating the non-conformal terms, the pQCD approximant becomes conformal series. As shown by Eqs.(17, 18), the C-scheme coupling $\hat{a}_\mu$ and the conventional coupling a_μ are mutually related by the RG-involved $\{\beta_i\}$-terms, thus the conformal coefficients $r_{i,0}$ at every order are the same for both cases.

- For an $n_{\rm th}$-order prediction, the effective conventional coupling $a_{Q_\star}$ satisfies the conventional RGE (1), which can be rewritten in the following form with the help of Eq.(43), i.e.

$$\frac{1}{a_{Q_\star}} + \frac{\beta_1}{\beta_0} \ln a_{Q_\star} = \beta_0 \left[\ln \frac{Q^2}{\Lambda^2} + \sum_{i\geq 0}^{\rm n-2} S_i a_{Q_\star}^i - \left(\int_0^{a_{Q_\star}} \frac{{\rm d}a}{\tilde{\beta}(a)} \right)_{\rm n-2} \right], \tag{57}$$

  where the subscript $(n-2)$ indicates the perturbative expansion is up to $a_{Q_\star}^{n-2}$-order. On the other hand, the effective C-scheme coupling $\hat{a}_{Q_\star}$ satisfies Eq.(55). By using the relation

$$\left(\int_0^{a_\mu} \frac{{\rm d}a}{\tilde{\beta}(a)} \right)_{n-2} = \sum_{i=1}^{\rm n-2} (S_i - \hat{S}_i) a_\mu^i, \tag{58}$$

  it can be further written as

$$\frac{1}{\hat{a}_{Q_\star}} + \frac{\beta_1}{\beta_0} \ln \hat{a}_{Q_\star} = \beta_0 \left[\ln \frac{Q^2}{\Lambda^2} + \sum_{i\geq 0}^{\rm n-2} S_i \hat{a}_{Q_\star}^i - \left(\int_0^{\hat{a}_{Q_\star}} \frac{{\rm d}a}{\tilde{\beta}(a)} \right)_{\rm n-2} \right]. \tag{59}$$

  Thus both the effective couplings $a_{Q_\star}$ and $\hat{a}_{Q_\star}$ are solutions of the same equation, Eq.(57) or Eq.(59), which can be solved iteratively. Those two equations are alternatives to the RGE, their solution is are identical for the choice of same scale Q, indicating $a_{Q_\star} \equiv \hat{a}_{Q_\star}$ for any fixed-order prediction.

IV. PHENOMENOLOGICAL EXAMPLES

In doing the numerical calculations below, we adopt the world average $\alpha_s^{\overline{\rm MS}}(M_Z) = 0.1181(11)$ (Patrignani *et al.*, 2016) as the reference value for fixing the running coupling, which runs down to $\alpha_s^{\overline{\rm MS}}(M_\tau) = 0.3159(95)$. $M_Z = 91.1876$ GeV and $M_\tau = 1.777$ GeV.

A. The non-singlet Adler function

The non-singlet Adler function (Adler, 1974) reads

$$D^{\rm ns}(Q^2,\mu) = 12\pi^2\left[\gamma^{\rm ns}(a_\mu) - \beta(a_\mu)\frac{\partial}{\partial a_\mu}\Pi^{\rm ns}(L,a_\mu)\right] = \frac{3}{4}\gamma_0^{\rm ns} + \bar{D}^{\rm ns}(Q^2,\mu), \tag{60}$$

where μ is the renormalization scale, $a_\mu = \alpha_s(\mu)/\pi$, and $L = \ln\mu^2/Q^2$. $\gamma^{\rm ns}(a_\mu) = \sum_{i\geq 0}\gamma_i^{\rm ns}a_\mu^i/16\pi^2$ is the non-singlet part of the photon field anomalous dimension and $\Pi^{\rm ns}(L,a_\mu) = \sum_{i\geq 0}\Pi_i^{\rm ns}a_\mu^i/16\pi^2$ is the non-singlet part of the polarization function for a flavor-singlet vector current. The pQCD series of $\bar{D}^{\rm ns}(Q^2,\mu)$ up to $n_{\rm th}$-loop level can be written as

$$\bar{D}_n^{\rm ns}(Q^2,\mu) = \sum_{i=1}^{n} r_i(\mu/Q)a_\mu^i. \tag{61}$$

The perturbative coefficients $\gamma_i^{\rm ns}$ and $\Pi_i^{\rm ns}$ within the $\overline{\rm MS}$-scheme have been given up to four-loop level (Baikov *et al.*, 2012a), and the coefficients r_i within the $\overline{\rm MS}$-scheme up to four-loop level can be read from Refs.(Baikov *et al.*, 2010; Chetyrkin *et al.*, 1996). For example, if setting $\mu = Q$ and $n_f = 3$, the first four $\overline{\rm MS}$-coefficients are

$$r_1 = 1,\ \ r_2 = 1.6398,\ \ r_3 = 6.3710,\ \ r_4 = 49.0757.$$

The coefficients at any other choices of the renormalization scale ($\mu \neq Q$) can be obtained via RGE.

1. Scheme-and-scale uncertainties using conventional scale-setting

Taking $Q = M_\tau$, we obtain a four-loop $\overline{\rm MS}$-scheme prediction on $\bar{D}^{\rm ns}$ using conventional scale-setting (Conv.),

$$\bar{D}_4^{\rm ns}(M_\tau^2,\mu = M_\tau)|_{\rm Conv.} = 0.1286 \pm 0.0053 \pm 0.0094\left({}^{+0.0257}_{-0.0109}\right), \tag{62}$$

where the first error is for $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$ and the second error is an estimate of the "unknown" high-order contribution, which is conservatively taken as the maximum value of the last known term of the perturbative series within the possible choices of initial scale (Wu *et al.*, 2015). As for the four-loop prediction, we take the maximum value of $|r_4(\mu/M_\tau)a_\mu^4|$ with $\mu \in [M_\tau, 4M_\tau]$ as the estimated "unknown" high-order contribution. We also present the conventional scale error predicted by varying $\mu \in [M_\tau/2, 2M_\tau]$ in the parenthesis, which gives $\bar{D}_4^{\rm ns}|_{\rm Conv.} \in [0.1265, 0.1543]$. The conventional scale error is still about 21% at the four-loop level. Thus a five-loop or even higher loop calculation is needed to suppress the scale uncertainty using the conventional scale setting approach.

The unknown fifth-order coefficient has been estimated by several groups, e.g. $r_5 \simeq 283$ (Beneke and Jamin, 2008) or $r_5 \simeq 275$ (Baikov *et al.*, 2008). If using $r_5 \simeq 283$, Eq.(62) changes to

$$\bar{D}_5^{\rm ns}(M_\tau^2,\mu = M_\tau)|_{\rm Conv.} = 0.1315 \pm 0.0057 \pm 0.0065\left({}^{-0.0052}_{-0.0079}\right), \tag{63}$$

which shows that the conventional scale uncertainty could be reduced to 6%.

In addition to the scale dependence, the predictions using conventional scale setting is also scheme dependent at any fixed order. We adopt the C-scheme coupling to illustrate this dependence.

By using the relation (17), we rewrite $\bar{D}_n^{\rm ns}(Q^2,\mu)$ in terms of the C-scheme coupling $\hat{a}_\mu$ as

$$\bar{D}_n^{\rm ns}(Q^2,C) = \sum_{i=1}^{n}\hat{c}_i(\mu/Q)\hat{a}_\mu^i, \tag{64}$$

where the coefficients $\hat{c}_i(\mu/Q)$ can be derived by using Eqs.(22, 23, 24, 25). For example, if setting $\mu = Q$ and $n_f = 3$, the C-dependent coefficients $\hat{c}_i$ in terms of r_i up to five-loop level are

$$\begin{aligned}
\hat{c}_1 &= 1, \;\; \hat{c}_2 = 1.6398 + 2.25C, \;\; \hat{c}_3 = 7.6816 + 11.3792C + 5.0625C^2, \\
\hat{c}_4 &= 61.0597 + 72.0804C + 47.4048C^2 + 11.3906C^3, \\
\hat{c}_5 &= r_5 + 65.4774 + 677.68C + 408.637C^2 + 162.464C^3 + 25.6289C^4.
\end{aligned}$$

Those coefficients at the NLO and higher orders explicitly depend on C.

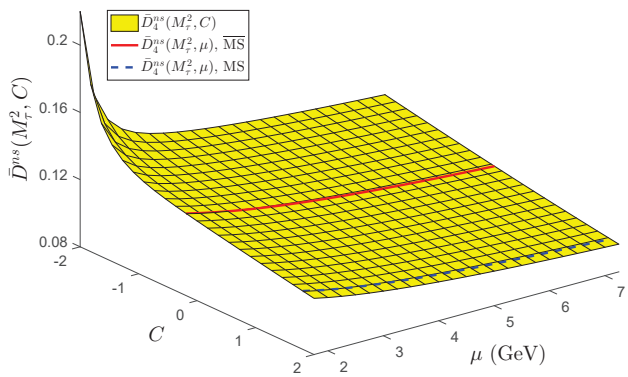

FIG. 2 (color online) The four-loop prediction on $\bar{D}^{\rm ns}(M_\tau^2, C)$ for the Adler function using conventional scale setting as a function of parameters C and μ, which is shown by a light shaded band. The solid line is for the $\overline{\rm MS}$-scheme, and the dashed line is for the MS-scheme.

A graphical representation of $\bar{D}^{\rm ns}(M_\tau^2, C)$ as a function of parameters C and μ is given in Fig. 2, in which we have chosen $C \in [-2, +2]$ [3] and $\mu \in [M_\tau, 4M_\tau]$. The light shaded band shows the four-loop prediction on $\bar{D}^{\rm ns}(M_\tau^2, C)$, which still shows a large scheme-and-scale dependence. Using a proper choice of C, the prediction using C-scheme coupling $\hat{a}_\mu$ are be equivalent to predictions using some of the familiar schemes; e.g. the solid line in Fig.2 is for the $\overline{\rm MS}$-scheme and the dashed line is for the MS-scheme. To ensure equivalence, the value of C should be changed for different scales. For example, by taking $C = -0.188$ one obtains the conventional $\overline{\rm MS}$ prediction for $\mu = M_\tau$; alternatively it can taken as $C = -0.004$ for $\mu = 4M_\tau$.

Requiring the estimated "unknown" high-order contribution, $|\hat{c}_n(\mu/M_\tau)\hat{a}_\mu^n|_{\rm MAX}$, to be at its minimum, we can obtain an optimal C-scheme for $\bar{D}_n^{\rm ns}(Q^2, C)$. At the four-loop level with $n = 4$, the optimal C-value is -0.972, leading to

$$\bar{D}_4^{\rm ns}(M_\tau^2, C = -0.972)|_{\rm Conv.} = 0.1365 \pm 0.0069 \pm 0.0083, \tag{65}$$

where the central value is for $\mu = M_\tau$, the first error is for $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$ and the second error is an estimate of the "unknown" high-order contribution. As for a five-loop prediction, if using $r_5 \simeq 283$, the optimal C-value changes to -1.129, and we obtain

$$\bar{D}_5^{\rm ns}(M_\tau^2, C = -1.129)|_{\rm Conv.} = 0.1338 \pm 0.0062 \pm 0.0054. \tag{66}$$

2. Predictions using PMC scale-setting

By applying PMC scale-setting, scheme and scale independent predictions can be achieved at any fixed order. To apply PMC scale-setting, we need to distribute the perturbative ones r_i into conformal coefficients ($r_{i,0}$) and non-conformal ones ($r_{i,j(\neq 0)}$), which can be achieved by using the β-pattern described by Eq.(30). Up to four-loop level, the known coefficients for conventional coupling are (Shen *et al.*, 2017b)

$$r_{i(\geq 1),0} = \frac{3}{4}\gamma_i^{\rm ns}, \;\; r_{i(\geq 2),1} = \frac{3}{4}\Pi_{i-1}^{\rm ns}, \;\; r_{i(\geq 3),2} = 0, \;\; r_{i(\geq 4),3} = 0. \tag{67}$$

[3] The relation between the C-scheme coupling $\hat{a}_{M_\tau}$ and the $\overline{\rm MS}$-scheme coupling a_{M_τ} ceases to be perturbative and breaks down below $C \sim -2$. Thus in our discussions we shall adopt $C \geq -2$.

Following the standard PMC single-scale approach, by resumming all the RG-involved non-conformal $\{\beta_i\}$-terms into the running coupling, we obtain the PMC prediction for $\bar{D}_n^{\rm ns}$, i.e.

$$\bar{D}_n^{\rm ns}(Q^2, C)|_{\rm PMC} = \frac{3}{4}\sum_{i=1}^{n}\gamma_i^{\rm ns}\hat{a}_{Q_\star}^i. \tag{68}$$

Using the known four-loop pQCD prediction $\bar{D}_4^{\rm ns}$, the PMC scale $Q_\star$ can be determined up to next-to-next-to-leading log (N^{2}LL) accuracy:

$$\ln\frac{Q_\star^2}{Q^2} = -C + 0.2249 - 3.1382\hat{a}_{Q_\star} - 13.3954\hat{a}_{Q_\star}^2, \tag{69}$$

in which the value of the C-scheme coupling $\hat{a}_{Q_\star}$ is determined by Eq.(55).

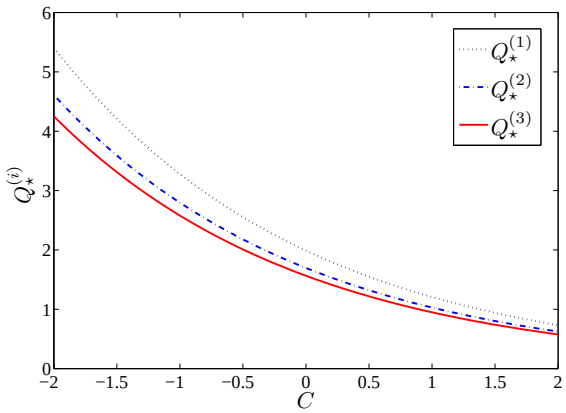

FIG. 3 The PMC scale $Q_\star^{(i)}$ of $\bar{D}_4^{\rm ns}(M_\tau^2, C)$ as a function of parameter C, where i indicates the scale is at the N$^{(i-1)}$LL accuracy.

The PMC scale $Q_\star$ is independent of the choice of the initial scale, consistent with the observation of Eq.(43); it is, however scheme-dependent, since it depends on the parameter C. We present $Q_\star$ as a function of C in Fig.3, in which $Q_\star^{(1,2,3)}$ are at the LL, NLL and N^{2}LL level, respectively. Fig.3 shows $Q_\star^{(1,2,3)}$ decreases with the increment of C, and $Q_\star^{(1)} > Q_\star^{(2)} > Q_\star^{(3)}$. The optimal scale $Q_\star$ is of perturbative nature: when more loop terms are included, it becomes more accurate. However, Eq.(55) shows that the C-scheme coupling at the scale Q^* ($\hat{a}_{Q_\star}$) is independent to the choice of C. By taking $Q = M_\tau$, we obtain $\hat{a}_{Q_\star} \equiv 0.1056(41)$ for any choice of C, where the errors are from $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$. We then obtain the scheme-independent PMC prediction on $\bar{D}_4^{\rm ns}$,

$$\bar{D}_4^{\rm ns}(M_\tau^2, C)|_{\rm PMC} = 0.1345 \pm 0.0066 \pm 0.0008, \tag{70}$$

where the first error is for $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$ and the second error is an estimate of the "unknown" high-order contribution, which equals to $\pm\left|\frac{3}{4}\gamma_4^{\rm ns}\hat{a}_{Q_\star}^4\right|$, since the PMC prediction is independent to the choice of initial scale μ.

In order to compare the scheme dependence before and after applying the PMC, we set the initial scale $\mu = M_\tau$, and present various predictions for $\bar{D}_4^{\rm ns}(M_\tau^2, C)$ in Fig. 4. The solid line is the prediction using conventional scale-setting, the lighter-shaded band shows the predicted unknown high-order contributions for various C values. At four-loop level, Fig. 4 shows that the scheme-dependence of $\bar{D}_4^{\rm ns}(M_\tau^2, C)|_{\rm Conv.}$ is rather large, which decreases with increasing values for C; for larger C values, the error band becomes slightly larger. When $C = -0.972$, the error bar is the minimum, corresponding to the optimal scheme. By further using the approximate five-loop term $r_5 \simeq 283$, we also give the results for the approximate five-loop prediction. Fig. 4 shows a smaller error bar is achieved with a five-loop term, $\bar{D}_5^{\rm ns}(M_\tau^2, C)|_{\rm Conv.}$ first increases and then decreases with the increment of C, and the optimal scheme is slightly shifted to $C = -1.129$. The flat dash-dot line in Fig. 4 shows that the conventional scheme dependence can be eliminated by applying the PMC. Due to the much faster pQCD convergence after applying the PMC, and due to the elimination of the scale dependence, the PMC suggests that the unknown high-order contribution could be quite small in comparison to the present four-loop prediction.

We present the value of each loop-term, LO, NLO, N^{2}LO, or N^{3}LO, for the four-loop prediction $\bar{D}_4^{\rm ns}$ using conventional (Conv.) and PMC scale-settings in Table I. Here κ_i stands for the ratio of the $i_{\rm th}$-order term over the total

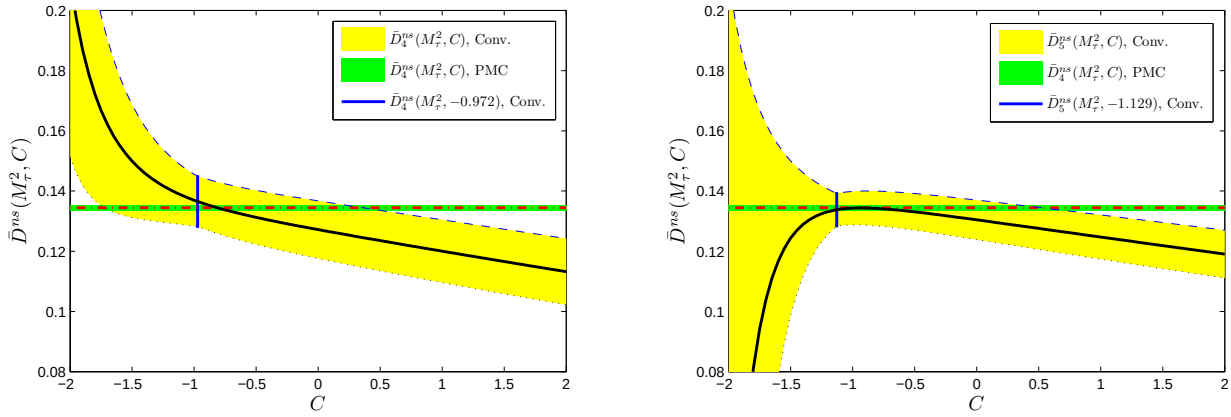

FIG. 4 (color online) $\bar{D}^{\rm ns}(M_\tau^2, C)$ for the Adler function as a function of the parameter C. The solid line is the prediction using conventional scale setting, the lighter-shaded band is the uncertainty for a four-loop prediction $\Delta = \pm|\hat{c}_4(\mu/M_\tau)\hat{a}_\mu^4|_{\rm MAX}$ (Left) and for an approximate five-loop prediction $\Delta = \pm|\hat{c}_5(\mu/M_\tau)\hat{a}_\mu^5|_{\rm MAX}$ (Right), where MAX is the maximum value for $\mu \in [M_\tau, 4M_\tau]$. When $C = -0.972$ (Left) and $C = -1.129$ (Right), the error bar as shown by a vertical solid line is the minimum. The dash-dot line represents the four-loop PMC prediction, and the darker shaded band is for $\Delta = \pm|\hat{r}_{4,0}\hat{a}_{Q_\star}^4|$. The independence of the PMC prediction on the parameter C demonstrates its scheme-independence.

TABLE I The value of each loop-term, LO, NLO, N^{2}LO, or N^{3}LO, for the four-loop prediction $\bar{D}_4^{\rm ns}$ using conventional (Conv.) and PMC scale-settings, respectively. $\mu = Q = M_\tau$. The results for the $\overline{\rm MS}$-scheme, the optimal C-scheme with $C = -0.972$, and the C-scheme with $C = -0.783$ (Boito *et al.*, 2016) are presented accordingly. The PMC prediction is unchanged for any choice of C-scheme. κ_i represents the relative importance among different orders.

	LO	NLO	N^{2}LO	N^{3}LO	Total	κ_1	κ_2	κ_3	κ_4
Conv., $\overline{\rm MS}$-scheme	0.1006	0.0166	0.0064	0.0050	0.1286	78%	13%	5%	4%
Conv.,$C = -0.783$	0.1254	-0.0019	0.0037	0.0070	0.1342	93%	-1%	3%	5%
Conv., optimal C-scheme	0.1347	-0.0099	0.0034	0.0083	0.1365	99%	-7%	2%	6%
PMC, any C-scheme	0.1056	0.0240	0.0041	0.0008	0.1345	79%	18%	3%	< 1%

contributions to $\bar{D}_4^{\rm ns}$, where $i = 1$ indicates the LO-order term, and etc.. The pQCD convergence for the conventional $\overline{\rm MS}$-scheme is moderate. The pQCD convergence for the optimal C-scheme ($C = -0.972$) does not suffer from the usual α_s-suppression, the relativity of the related high-loop terms show, $|\bar{D}_4^{\rm ns,LO}| \gg |\bar{D}_4^{\rm ns,NLO}| \sim |\bar{D}_4^{\rm ns,N^2LO}| \sim |\bar{D}_4^{\rm ns,N^3LO}|$. On the other hand, by applying the PMC, a much better pQCD convergence is naturally achieved due to the elimination of the divergent renormalon-like terms.

An approximate method to determine the optimal C-scheme is suggested in Ref.(Boito *et al.*, 2016) by fixing the renormalization scale $\mu = Q$ and requiring the magnitude of the last known-term $\hat{c}_n(Q/Q)\hat{a}_Q^n$ to be at its minimum. Using this suggestion, the uncertainty is assumed to be given by the magnitude of $\hat{c}_n(Q/Q)\hat{a}_Q^n$, and if specifically $\hat{c}_n(Q/Q)\hat{a}_Q^n$ equals to zero for an optimal C, one sets the one-order lower term $\hat{c}_{n-1}(Q/Q)\hat{a}_Q^{n-1}$ as the uncertainty. Fig.5 shows $\bar{D}_5^{\rm ns}(M_\tau^2, C)$ as a function of C for $\mu = Q = M_\tau$ by using the approximate five-loop term $r_5 \simeq 283$; its predicted optimal C is -0.783, which leads to $|\hat{c}_5(M_\tau/M_\tau)\hat{a}_{M_\tau}^5| = 0$ and $\bar{D}_5^{\rm ns}(M_\tau^2, C = -0.783)|_{\rm Conv.} = 0.1342 \pm 0.0063 \pm 0.0070$, where the first error is for $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$ and the second error is equals to $\pm|\hat{c}_4(M_\tau/M_\tau)\hat{a}_{M_\tau}^4|$.

B. τ decays to $\nu+$ hadrons

The ratio of the τ total hadronic branching fraction to its lepton branching fraction can be parameterized as,

$$R_\tau = \frac{\Gamma(\tau \to {\rm hadrons} + \nu_\tau)}{\Gamma(\tau \to l + \bar{\nu}_l + \nu_\tau)} = 3S_{\rm EW}\left(|V_{ud}|^2 + |V_{us}|^2\right)(1 + \delta^{(0)} + \cdots), \tag{71}$$

where $S_{\rm EW}$ is an electroweak correction, $|V_{ud}|$ as well as $|V_{us}|$ are CKM matrix elements. The pQCD correction is encoded in $\delta^{(0)}$ and the ellipsis indicate further small subleading corrections. The pQCD correction up to $n_{\rm th}$-order

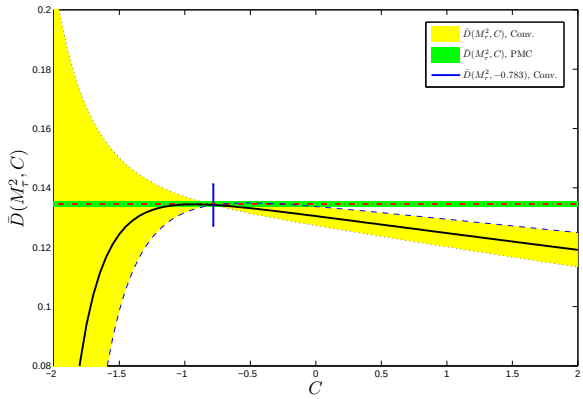

FIG. 5 (color online) $\bar{D}^{\rm ns}(M_\tau^2, C)$ as a function of C using conventional scale-setting, which agrees with that of Ref.(Boito *et al.*, 2016). $\mu = Q = M_\tau$. The solid line is the approximate five-loop prediction with $r_5 \simeq 283$ using conventional scale setting, the lighter-shaded band is its uncertainty $\Delta = \pm\hat{c}_5(M_\tau/M_\tau)\hat{a}^5_{M_\tau}$. The optimal scheme corresponds to $C = -0.783$, which leads to a vanishing $\hat{c}_5(M_\tau/M_\tau)\hat{a}^5_{M_\tau}$, and $\pm|\hat{c}_4(M_\tau/M_\tau)\hat{a}^4_{M_\tau}|$ is taken as its uncertainty. As a comparison, the dash-dot line represents the scheme-independent four-loop PMC prediction, whose darker-shaded band is for $\Delta = \pm|\hat{r}_{4,0}\hat{a}^4_{Q_\star}|$.

level reads,

$$\delta^{(0)}_n(M_\tau^2, \mu) = \sum_{i=1}^{n} c_i(\mu/M_\tau)a^i_\mu, \tag{72}$$

where the perturbative coefficients c_i for the $\overline{\rm MS}$-scheme up to four-loop level can be found in Refs.(Beneke and Jamin, 2008; Baikov *et al.*, 2008). Numerically, the first five coefficients c_i for $\mu = M_\tau$ and $n_f = 3$ are,

$$c_1 = 1,\ \ c_2 = 5.2023,\ \ c_3 = 26.3659,\ \ c_4 = 127.079,\ \ c_5 = 307.783 + r_5.$$

1. Scheme-and-scale uncertainties using conventional scale-setting

Taking $\mu = M_\tau$, we obtain a four-loop $\overline{\rm MS}$-scheme prediction on $\delta^{(0)}$ using conventional scale-setting (Conv.),

$$\delta^{(0)}_4(M_\tau^2, \mu = M_\tau)|_{\rm Conv.} = 0.1930 \pm 0.0104 \pm 0.0199\left({}^{+0.0169}_{-0.0285}\right), \tag{73}$$

where the first error is for $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$ and the second error is an estimate of the "unknown" high-order contribution. We also present the conventional scale error predicted by varying $\mu \in [M_\tau/2, 2M_\tau]$ in the parenthesis, which gives $\delta^{(0)}_4|_{\rm Conv.} \in [0.1645, 0.2099]$. The scale error using conventional scale setting is $\sim 15\%$ at the four-loop level. If we use the predicted five-loop term $r_5 \simeq 283$ (Beneke and Jamin, 2008) , we obtain

$$\delta^{(0)}_5(M_\tau^2, \mu = M_\tau)|_{\rm Conv.} = 0.1990 \pm 0.0113 \pm 0.0151\left({}^{-0.0053}_{-0.0202}\right), \tag{74}$$

it shows the conventional scale uncertainty is still large $\sim 10\%$.

The predictions using conventional scale setting are scheme dependent. By using the relation (17), we rewrite $\delta^{(0)}_n(M_\tau^2, \mu)$ in terms of the C-scheme coupling $\hat{a}_\mu$ as

$$\delta^{(0)}_n(M_\tau^2, C) = \sum_{i=1}^{n} \hat{c}_i(\mu/M_\tau)\hat{a}^i_\mu, \tag{75}$$

where the first five coefficients for $\mu = M_\tau$ and $n_f = 3$ reads,

$$\begin{aligned}
\hat{c}_1 &= 1,\ \ \hat{c}_2 = 5.2023 + 2.25C,\ \ \hat{c}_3 = 27.6765 + 27.4104C + 5.0625C^2,\\
\hat{c}_4 &= 148.4 + 235.546C + 101.51C^2 + 11.3906C^3,\\
\hat{c}_5 &= 198.853 + 1754.35C + 1240.42C^2 + 324.781C^3 + 25.6289C^4 + c_5.
\end{aligned}$$

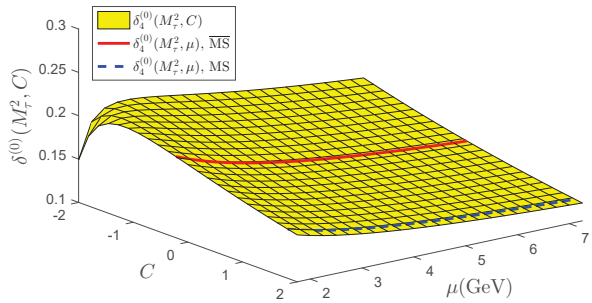

FIG. 6 (color online) The four-loop prediction on $\delta^{(0)}(M_\tau^2, C)$ using conventional scale setting as a function of parameters C and μ, which is shown by a light shaded band. The solid line is for the $\overline{\rm MS}$-scheme, and the dashed line is for the MS-scheme.

A graphical representation of $\delta^{(0)}(M_\tau^2, C)$ as a function of parameters C and μ is given in Fig. 2, in which we have chosen $C \in [-2, +2]$ and $\mu \in [M_\tau, 4M_\tau]$. The light shaded band shows the four-loop prediction on $\delta^{(0)}(M_\tau^2, C)$, the solid line is $\overline{\rm MS}$-scheme prediction and the dashed line is the MS-scheme one.

Requiring the approximate "unknown" high-order contribution, $|\hat{c}_n(\mu/M_\tau)\hat{a}_\mu^n|_{\rm MAX}$, minimal, we obtain an optimal C-scheme for $\delta^{(0)}(M_\tau^2, C)$ at the $n_{\rm th}$-order level. Using the four-loop prediction with $n = 4$, the optimal C-value is -1.638, which leads to

$$\delta_4^{(0)}(M_\tau^2, C = -1.638)|_{\rm Conv.} = 0.1979 \pm 0.0099 \pm 0.0186. \tag{76}$$

where the first error is for $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$, and the second error is for $\pm|\hat{c}_4(\mu/M_\tau)\hat{a}_\mu^4|_{\rm MAX}$. If using the five-loop term $r_5 \simeq 283$, the optimal C-value changes to -1.813, and we obtain

$$\delta_5^{(0)}(M_\tau^2, C = -1.813)|_{\rm Conv.} = 0.1968 \pm 0.0095 \pm 0.0118. \tag{77}$$

2. Predictions for τ decay using PMC scale-setting

By applying PMC scale-setting, it is found that a scheme and scale independent prediction can be achieved at any fixed order. Up to four-loop level, the known conformal and non-conformal coefficients for conventional coupling are (Brodsky *et al.*, 2014),

$$\begin{aligned} r_{i(\geq 1),0} &= \frac{3}{4}\gamma_i^{\rm ns}, \;\; r_{i(\geq 2),1} = \frac{19}{256}\gamma_{i-1}^{\rm ns} + \frac{3}{64}\Pi_{i-1}^{\rm ns}, \\ r_{i(\geq 3),2} &= \left(\frac{265}{6144} - \frac{\pi^2}{256}\right)\gamma_{i-2}^{\rm ns} + \frac{19}{512}\Pi_{i-2}^{\rm ns}, \;\; r_{i(\geq 4),3} = \left(\frac{3355}{98304} - \frac{19\pi^2}{4096}\right)\gamma_{i-3}^{\rm ns} + \left(\frac{265}{8192} - \frac{3\pi^2}{1024}\right)\Pi_{i-3}^{\rm ns}. \end{aligned} \tag{78}$$

By resumming all the RG-involved non-conformal $\{\beta_i\}$-terms into the running coupling, we obtain the PMC prediction for $\delta_n^{(0)}(M_\tau^2, C)$, i.e.

$$\delta_n^{(0)}(M_\tau^2, C)|_{\rm PMC} = \frac{3}{4}\sum_{i=1}^{n}\gamma_i^{\rm ns}\hat{a}_{Q_\star}^i, \tag{79}$$

Using the known four-loop pQCD prediction $\delta_4^{(0)}(M_\tau^2, C)$, the PMC scale $Q_\star$ can be determined up to next-to-next-to-leading log (N^{2}LL) accuracy:

$$\ln\frac{Q_\star^2}{M_\tau^2} = -C - 1.3584 + 1.6234\hat{a}_{Q_\star} - 1.1385\hat{a}_{Q_\star}^2, \tag{80}$$

where the optimal C-scheme coupling $\hat{a}_{Q_\star}$ is determined by Eq.(55).

We present the scheme-dependent $Q_\star$ as a function of C in Fig.7, in which $Q_\star^{(1,2,3)}$ are at the LL, NLL and N^{2}LL level, respectively. To compare with the case of $\bar{D}^{\rm ns}(Q^2)$, the perturbative series for $\ln Q_\star^2/M_\tau^2$ oscillates, leading to

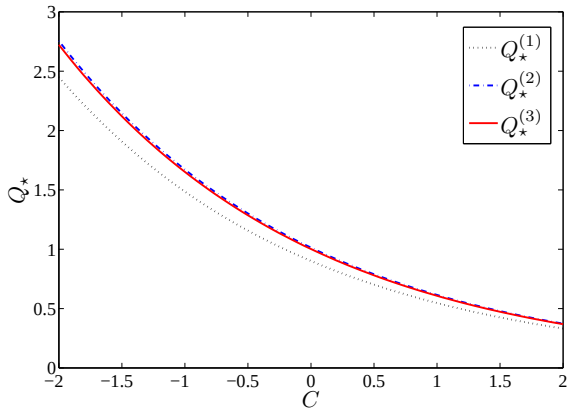

FIG. 7 The PMC scale $Q_\star^{(i)}$ of $\delta_4^{(0)}(M_\tau^2, C)$ as a function of parameter C, where i indicates the scale is at the $\mathrm{N}^{(i-1)}$LL accuracy.

$Q_\star^{(1)} < Q_\star^{(2)}$ and $Q_\star^{(2)} > Q_\star^{(3)}$; similar to the case of $\bar{D}^{\rm ns}(Q^2)$, $Q_\star^{(1,2,3)}$ decreases with increasing C; the prediction will become more precise when more loop terms are included. Eq.(55) indicates the C-scheme coupling $\hat{a}_{Q_\star}$ is free of the parameter C, and for the four-loop level we obtain $\hat{a}_{Q_\star} = 0.1449(63)$, where the error is for $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$. We then obtain the scheme-and-scale independent PMC prediction on $\delta_4^{(0)}(M_\tau^2, C)$,

$$\delta_4^{(0)}(M_\tau^2, C)|_{\rm PMC} = 0.2035 \pm 0.0123 \pm 0.0030. \tag{81}$$

where the first error is for $\Delta\alpha_s^{\overline{\rm MS}}(M_Z) = \pm 0.0011$ and the second error is an estimate of the "unknown" high-order contribution, which is $\pm\left|\frac{3}{4}\gamma_4^{\rm ns}\hat{a}_{Q_\star}^4\right|$.

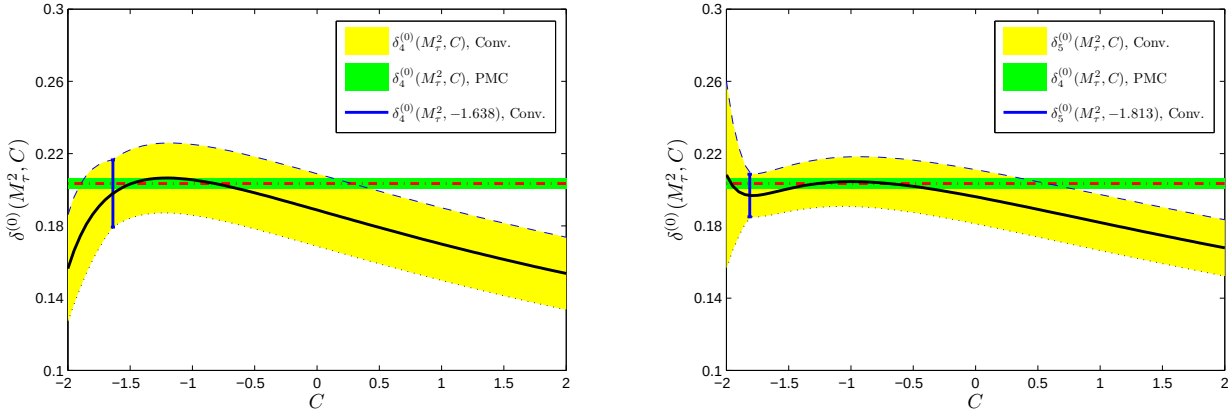

FIG. 8 (color online) $\delta^{(0)}(M_\tau^2, C)$ for τ decay as a function of the parameter C. The solid line is the prediction using conventional scale setting, the lighter-shaded band is the uncertainty for a four-loop prediction $\Delta = \pm|\hat{c}_4(\mu/M_\tau)\hat{a}_\mu^4|_{\rm MAX}$ (Left) and for an approximate five-loop prediction $\Delta = \pm|\hat{c}_5(\mu/M_\tau)\hat{a}_\mu^5|_{\rm MAX}$ (Right), where MAX is the maximum value for $\mu \in [M_\tau, 4M_\tau]$. When $C = -1.638$ (Left) and $C = -1.183$ (Right), the error bar as shown by a vertical solid line is the minimum. The dash-dot line represents the four-loop PMC prediction, and the darker shaded band is for $\Delta = \pm|\hat{r}_{4,0}\hat{a}_{Q_\star}^4|$. The independence of the PMC prediction on the parameter C demonstrates its scheme-independence.

To compare the scheme dependence before and after applying the PMC, we set the initial scale $\mu = M_\tau$, and present various predictions on $\delta^{(0)}(M_\tau^2, C)$ in Fig. 8. The solid line is the prediction using conventional scale-setting, the lighter-shaded band shows the predicted unknown high-order contributions for various C values. At four-loop level, Fig. 8 shows that the error band shall first increases and then decreases with increasing C; the optimal scheme is obtained for $C = -1.638$. By further using the approximate five-loop term $r_5 \simeq 283$, we give the results for the approximate five-loop prediction. Fig. 8 shows a smaller error bar is achieved with a five-loop term, $\bar{D}_5^{\rm ns}(M_\tau^2, C)|_{\rm Conv.}$ oscillates with the increment of C, and the optimal scheme is slightly shifted to $C = -1.813$. The flat dash-dot line in

Fig. 8 shows the conventional scheme dependence can be eliminated by applying the PMC. The unknown high-order contribution could be quite small for the present four-loop PMC prediction.

TABLE II The value of each loop-term, LO, NLO, N^{2}LO, or N^{3}LO, for the four-loop prediction $\delta_4^{(0)}(M_\tau^2)$ using conventional (Conv.) and PMC scale-settings, respectively. $\mu = Q = M_\tau$. The results for the $\overline{\rm MS}$-scheme, the optimal C-scheme with $C = -1.638$, and the C-scheme with $C = -0.882$ (Boito *et al.*, 2016) are presented accordingly. The PMC prediction is unchanged for any choice of C-scheme. κ_i represents the relative importance among different orders.

	LO	NLO	N^{2}LO	N^{3}LO	Total	κ_1	κ_2	κ_3	κ_4
Conv., $\overline{\rm MS}$-scheme	0.1006	0.0526	0.0268	0.0130	0.1930	52%	27%	14%	7%
Conv., $C = -0.882$	0.1301	0.0544	0.0164	0.0034	0.2043	64%	27%	8%	2%
Conv., optimal C-scheme	0.1873	0.0532	−0.0240	−0.0186	0.1979	95%	27%	−12%	−10%
PMC, any C-scheme	0.1449	0.0451	0.0105	0.0030	0.2035	71%	22%	5%	2%

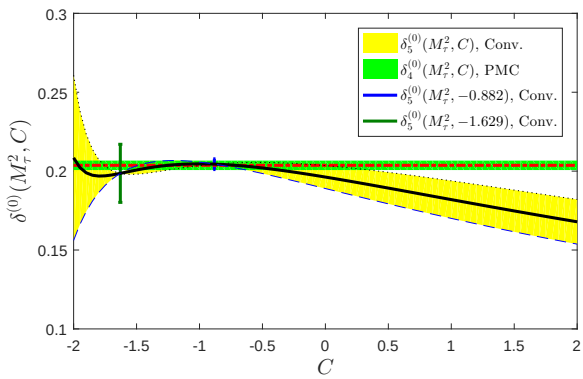

FIG. 9 (color online) $\delta^{(0)}(M_\tau^2, C)$ as a function of C, with $\mu = M_\tau$. The solid line is the approximate five-loop prediction using conventional scale setting, the lighter-shaded band is the uncertainty $\Delta = \pm\hat{c}_5(M_\tau/M_\tau)\hat{a}^5_{M_\tau}$. In the cross-point, $C = -1.629$ or $C = -0.882$, $\hat{c}_5(M_\tau/M_\tau)\hat{a}^5_{M_\tau}$ vanishes, and $\pm|\hat{c}_4(M_\tau/M_\tau)\hat{a}^4_{M_\tau}|$ is taken as the uncertainty. The dash-dot line represents the scheme-independent four-loop PMC prediction, whose darker-shaded band is for $\Delta = \pm|\hat{r}_{4,0}\hat{a}^4_{Q_\star}|$.

We present the value of each loop-term, LO, NLO, N^{2}LO, or N^{3}LO, for the four-loop prediction $\delta_4^{(0)}$ using conventional (Conv.) and PMC scale-settings in Table II. Here κ_i stands for the ratio of the $i_{\rm th}$-order term over the total contributions to $\delta_4^{(0)}$, where $i = 1$ indicates the LO-order term, etc. The pQCD convergence for the conventional $\overline{\rm MS}$-scheme is moderate. The pQCD convergence for the optimal C-scheme ($C = -1.638$) does not suffer from the usual α_s-suppression, $|\delta_4^{(0),{\rm LO}}| \gg |\delta_4^{(0),{\rm NLO}}| \sim |\delta_4^{(0),{\rm N^2LO}}| \sim |\delta_4^{(0),{\rm N^3LO}}|$. On the other hand, by applying the PMC, a much better pQCD convergence is naturally achieved due to the elimination of divergent renormalon-like terms. The value of $C = -0.882$ is determined by fixing the renormalization scale $\mu = Q$ and requiring the magnitude of the last known-term $\hat{c}_5(Q/Q)\hat{a}^n_Q$ to be the minimum (Boito *et al.*, 2016). Fig.9 shows $\delta_5^{(0)}(M_\tau^2, C)$ as a function of C for $\mu = Q = M_\tau$ by using the approximate five-loop term $r_5 \simeq 283$; its predicted optimal C is -0.882. Fig.9 shows there are two C values, $C = -1.629$ and $C = -0.882$, lead to $\hat{c}_5(M_\tau/M_\tau)\hat{a}^5_{M_\tau} = 0$, and the optimal scheme is chosen for $C = -0.882$ which has a minimum value for $|\hat{c}_4(M_\tau/M_\tau)\hat{a}^4_{M_\tau}|$. We note the conventional prediction with $C = -0.882$ is in agreement with the PMC prediction; a similar pQCD convergence has also been observed in Table II. Thus the PMC provides an underlying reason for the correctness of the optimal scheme for a high-order prediction using conventional scale-setting.

V. SUMMARY

We have shown that the scheme-and-scale ambiguities introduced by conventional scale-setting are unnecessary by combining the single-scale PMC procedure with the newly suggested scheme-independent C-scheme coupling. We have demonstrated that using the C=-scheme, together with the single-scale PMC-s, leads to perturbative QCD predictions which are explicitly independent of the initial renormalization scale and the choice of the renormalization scheme at all orders.

This method for eliminating the scale and scheme ambiguities relies heavily on how well we know the precise value and analytic properties of of the strong coupling α_s. An extended RGE can be adopted to determine the α_s scheme-and-scale running behaviors simultaneously; however, these dependences are usually entangled with each other and can only be solved perturbatively or numerically. In contrast, the scheme-and-scale running behavior of a C-scheme coupling $\hat{\alpha}_s$ can be exactly separated; it satisfies a RGE free of scheme-dependent $\{\beta_{i\geq 2}\}$-terms. The choice of the parameter C is chosen to match a conventional coupling α_s. The resulting scheme-independent RGE for the C-scheme coupling $\hat{\alpha}_s$ provides scheme-independent predictions. In fact, by using the C-scheme coupling, we have shown that explicitly scheme-independent predictions are obtained for any choice of the renormalization scheme for the conventional coupling.

Perturbative QCD predictions based on PMC scale setting satisfy the standard RGI and all the self-consistency conditions of the renormalization group. Because the divergent renormalon terms are eliminated, the convergence of the PMC series depends on conformal coefficients which are more convergent than conventional pQCD series. The PMC utilizes the RGE recursively to identify the occurrence and pattern of nonconformal $\{\beta_i\}$-terms in a pQCD expansion. The PMC scales are then fixed at each order, as in Gell-Mann-Low scale setting for QED. We can also extend the PMC method to assign a single effective renormalization scale for all orders. The resulting PMC single-scale approach not only makes the implementation and automation of PMC scale-setting simpler and more transparent, but it also achieves precise scheme-and-scale independent predictions simultaneously. As shown by Eqs.(43, 51), the $(\ln Q_*^2/\ln Q^2)$ expansion coefficients S_i and $\hat{S}_i$ do not depend on the initial renormalization scale μ; thus the PMC and PMC-s predictions are not only scheme independent, but also free of the choice for μ.

As we have shown, one can utilize a novel *C-scheme* coupling (Boito *et al.*, 2016) whose scheme-and-scale running behaviors are both governed by a single RGE which is free of scheme-dependent $\{\beta_{i\geq 2}\}$-terms. The value of the parameter C can be chosen to match any conventional renormalization scheme By using the C-scheme coupling instead of the conventional coupling, we have demonstrated that the C-dependence of the PMC predictions can be eliminated up to any fixed order; since the value of C is arbitrary, it means the PMC prediction is independent of any renormalization scheme. The approach is independent of the specific use of dimensional regularization. Two four-loop PMC examples confirm these observations. Thus combining the C-scheme coupling with the PMC single-scale approach (PMC-s), the resulting predictions become completely independent of the choice of the renormalization scheme and the initial renormalization scale, thus satisfying all of the conditions of RGI.

The PMC procedure thus systematically eliminates the scheme and scale ambiguities of pQCD predictions, greatly improving the precision of tests of the Standard Model and the sensitivity of collider experiments to new physics. Furthermore, since the perturbative coefficients obtained using the PMC are identical to those of a conformal theory, one can derive all-orders commensurate scale relations between physical observables evaluated at specific relative scales. An example is the Generalized Crewther Relation, which shows that the product of $R_{e^+e^-}(s)$ times the integral over the spin-dependent structure functions $g_1(x, Q^2)$ which enters the Bjorken sum rule at a specific value of Q^2/s has no leading-twist radiative QCD corrections at all orders.

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References

Brodsky, S.J., Lepage, G.P., Mackenzie, P.B., 1983, Phys. Rev. D **28**, 228.
Grunberg, G., 1980, Phys. Lett. B **95**, 70.
Grunberg, G., 1984, Phys. Rev. D **29**, 2315.
Stevenson, P.M., 1981, Phys. Lett. B **100**, 61.
Stevenson, P.M., 1981, Phys. Rev. D **23**, 2916.
Stevenson, P.M., 1982, Nucl. Phys. B **203**, 472.
Stevenson, P.M., 1984, Nucl. Phys. B **231**, 65.
Beneke, M., 1999, Phys. Rept. **317**, 1.
Gardi, E., Grunberg, G., 2001, Phys. Lett. B **517**, 215.
Bogoliubov, N.N., Shirkov, D.V., 1955, Dok. Akad. Nauk SSSR **103**, 391.
Callan, C.G., 1970, Phys. Rev. D **2**, 1541.
Peterman, A., 1979, Phys. Rep. **53**, 157.
Stuckelberg, E.C.G., Peterman, A., 1953, Helv. Phys. Acta **26**, 499.
Symanzik, K., 1970, Commun. Math. Phys. **18**, 227.
Wu, X.G., Brodsky, S.J., Mojaza, M., 2013, Prog. Part. Nucl. Phys. **72**, 44.

Brodsky, S.J. and Wu, X.G., 2012, Phys. Rev. D **85**, 034038.
Brodsky, S.J. and Giustino, L.Di, 2012, Phys. Rev. D **86**, 085026.
Mojaza, M., Brodsky, S.J., Wu, X.G., 2013, Phys. Rev. Lett. **110**, 192001.
Brodsky, S.J., Mojaza, M., Wu, X.G., 2014, Phys. Rev. D **89**, 014027.
Lu, H.J., Brodsky, S.J., 1993, Phys. Rev. D **48**, 3310.
Brodsky, S.J. and Wu, X.G., 2012, Phys. Rev. Lett. **109**, 042002.
Brodsky, S.J. and Wu, X.G., 2012, Phys. Rev. D **86**, 014021.
Chetyrkin, K.G., Kniehl, B.A., Steinhauser, M., 1997, Phys. Rev. Lett. **79**, 2184.
Gell-Mann, M. and Low, F.E., 1954, Phys. Rev. **95**, 1300.
Brodsky, S.J., Huet, P., 1998, Phys. Lett. B **417**, 145.
Brodsky, S.J. and Wu, X.G., 2012, Phys. Rev. D **86**, 054018.
Gross, D.J. and Wilczek, F., 1973, Phys. Rev. Lett. **30**, 1343.
Politzer, H.D., 1973, Phys. Rev. Lett. **30**, 1346.
Caswell, W.E., 1974, Phys. Rev. Lett. **33**, 244.
Tarasov, O.V., Vladimirov, A.A., Zharkov, A. Yu, 1997, Phys. Lett. B **93**, 429.
Larin, S.A., Vermaseren, J.A.M., 1993, Phys. Lett. B **303**, 334.
Ritbergen, T. van, Vermaseren, J.A.M., Larin, S.A., 1997, Phys. Lett. B **400**, 379.
Chetykin, K.G., 2005, Nucl. Phys. B **710**, 499.
Czakon, M., 2005, Nucl. Phys. B **710**, 485.
Baikov, P.A., Chetyrkin, K.G., Kuhn, J.H., 2017, Phys. Rev. Lett. **118**, 082002.
Patrignani, C., *et al.* (Particle Data Group), 2016, Chin. Phys. C **40**, 100001.
Celmaster, W., Gonsalves, R.J., 1978, Phys. Rev. D **20**, 1420.
Celmaster, W., Gonsalves, R.J., 1979, Phys. Rev. Lett. **42**, 1435.
Zeng, D.M., Wang, S.Q., Wu, X.G., Shen, J.M., 2016, J. Phys. G **43**, 075001.
Boito, D., Jamin, M., Miravitllas, R., 2016, Phys. Rev. Lett. **117**, 152001.
Brodsky, S.J., Lu, H.J., 1993, Phys. Rev. D **51**, 3652.
Shen, J.M., Wu, X.G., Ma, Y., Brodsky, S.J., 2017, Phys. Lett. B **770**, 494.
Broadhurst, D.J., Kataev, A.L., 1993, Phys. Lett. B **315**, 179.
Brodsky, S.J., Gabadadze, G.T., Kataev, A.L., Lu, H.J., 1996, Phys. Lett. B **372**, 133.
Crewther, R.J., 1997, Phys. Lett. B **397**, 137.
Corless, R.M., Gonnet, G.H., Hare, D.E.G., Jeffrey, D.J., Knuth, D.E., 1996, Adv. Comput. Math. **5**, 329.
't Hooft, G., 1977, in the Proceedings of the International School of Subnuclear Physics, Erice, Italy, 1977, edited by A. Zichichi, Subnuclear series Vol. 15 (Plenum, New York, 1979), p. 943.
Jamin, M. and Miravitllas, R., 2016, JHEP **1610**, 059.
Ma, Y., Wu, X.G., Ma, H.H., Han, H.Y., 2015, Phys. Rev. D **91**, 034006.
Wu, X.G., Ma, Y., Wang, S.Q., Fu, H.B., Ma, H.H., Brodsky, S.J., Mojaza, M., 2015, Rep. Prog. Phys. **78**, 126201.
Bi, H.Y., Wu, X.G., Ma, Y., Ma, H.H., Brodsky, S.J., Mojaza, M., 2015, Phys. Lett. B **748**, 13.
Shen, J.M., Wu, X.G., Du, B.L., Brodsky, S.J., 2017, Phys. Rev. D **95**, 094006.
Deur, A., Shen, J.M., Wu, X.G., Brodsky, S.J., de Teramond, G.F., 2017, Phys. Lett. B **773**, 98.
Brodsky, S.J., Hwang, D.S., Schmidt, I., 2002, Phys. Lett. B **530**, 99.
Brodsky, S.J., Hwang, D.S., Boer, D., 2003, Phys. Rev. D **67**, 054003.
Adler, S.L., 1974, Phys. Rev. D **10**, 3714.
Baikov, P.A., Chetyrkin, K.G., Kuhn, J.H., Rittinger, J., 2012, JHEP **1207**, 017.
Baikov, P.A., Chetyrkin, K.G., Kuhn, J.H., 2010, Phys. Rev. Lett. **104**, 132004.
Chetyrkin, K.G., Kuhn, J.H., Kwiatkowski, A., 1996, Phys. Rept. **277**, 189.
Beneke, M. and Jamin, M., 2008, JHEP **0809**, 044.
Baikov, P.A., Chetyrkin, K.G., Kuhn, J.H., 2008, Phys. Rev. Lett. **101**, 012002.