



Systematic All-Orders Method to Eliminate Renormalization-Scale and Scheme Ambiguities in Perturbative QCD

Matin Mojaza*

*CP3-Origins, Danish Institute for Advanced Studies, University of Southern Denmark, DK-5230 Odense, Denmark
and SLAC National Accelerator Laboratory, Stanford University, Stanford, California 94039, USA*

Stanley J. Brodsky†

SLAC National Accelerator Laboratory, Stanford University, Stanford, California 94039, USA

Xing-Gang Wu‡

Department of Physics, Chongqing University, Chongqing 401331, People's Republic of China

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We introduce a generalization of the conventional renormalization schemes used in dimensional regularization, which illuminates the renormalization scheme and scale ambiguities of perturbative QCD predictions, exposes the general pattern of nonconformal $\{\beta_i\}$ terms, and reveals a special degeneracy of the terms in the perturbative coefficients. It allows us to systematically determine the argument of the running coupling order by order in perturbative QCD in a form which can be readily automatized. The new method satisfies all of the principles of the renormalization group and eliminates an unnecessary source of systematic error.

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An important goal in high energy physics is to make perturbative QCD (pQCD) predictions as precise as possible, not only to test QCD itself, but also to expose new physics beyond the standard model. In this Letter we present a systematic method which determines the argument of the running coupling order by order in pQCD and which can be readily automatized. The resulting predictions for physical processes are independent of theoretical conventions such as the choice of renormalization scheme and the initial choice of renormalization scale. The resulting scales also determine the effective number of quark flavors at each order of perturbation theory. The method can be applied to processes with multiple physical scales and is consistent with QED scale setting in the limit $N_c \rightarrow 0$. The new method satisfies all of the principles of the renormalization group [1], and it eliminates an unnecessary source of systematic error.

The starting point for our analysis is to introduce a generalization of the conventional schemes used in dimensional regularization in which a constant $-\delta$ is subtracted in addition to the standard subtraction $\ln 4\pi - \gamma_E$ of the $\overline{\text{MS}}$ scheme. This amounts to redefining the renormalization scale by an exponential factor; i.e., $\mu_\delta^2 = \mu_{\overline{\text{MS}}}^2 \exp(\delta)$. In particular, the $\overline{\text{MS}}$ scheme is recovered for $\delta = \ln 4\pi - \gamma_E$. The δ subtraction defines an infinite set of renormalization schemes which we call δ - \mathcal{R} enormalization (\mathcal{R}_δ) schemes; since physical results cannot depend on the choice of scheme, predictions must be independent of δ . Moreover, since all \mathcal{R}_δ schemes are connected by scale displacements, the β function of the strong QCD coupling constant $a = \alpha_s/4\pi$ is the same in any \mathcal{R}_δ scheme:

$$\mu_\delta^2 \frac{da}{d\mu_\delta^2} = \beta(a) = -a(\mu_\delta)^2 \sum_{i=0}^{\infty} \beta_i a(\mu_\delta)^i. \quad (1)$$

The \mathcal{R}_δ scheme exposes the general pattern of nonconformal $\{\beta_i\}$ terms, and it reveals a special degeneracy of the terms in the perturbative coefficients which allows us to resum the perturbative series. The resummed series matches the conformal series, which is itself free of any scheme and scale ambiguities as well as being free of a divergent renormalon series. It is the final expression one should use for physical predictions. It also makes it possible to set up an algorithm for automatically computing the conformal series and setting the effective scales for the coupling constant at each perturbative order.

Consider an observable in pQCD in some scheme which we put as the reference scheme \mathcal{R}_0 (e.g., the $\overline{\text{MS}}$ scheme, which is the conventional scheme used) with the following expansion:

$$\rho_0(Q^2) = \sum_{i=0}^{\infty} r_i(Q^2/\mu_0^2) a(\mu_0)^i, \quad (2)$$

where μ_0 stands for the initial renormalization scale and Q is the kinematic scale of the process. The more general expansion with higher Born-level power in a can be readily derived [2] and will not change our conclusions and results. The full pQCD series is formally independent of the choice of the initial renormalization scale μ_0 , if it were possible to sum the entire series. However, this goal is not feasible in practice, especially because of the $n! \beta^n \alpha_s^n$ renormalon growth of the nonconformal series. When a perturbative expansion is truncated at any finite order, it generally

becomes renormalization-scale and scheme dependent, i.e., dependent on theoretical conventions. This can be exposed by using the \mathcal{R}_δ scheme. Since results in any \mathcal{R}_δ are related by scale displacements, we can derive a general expression for ρ by using the displacement relation between couplings in any \mathcal{R}_δ scheme:

$$a(\mu_0) = a(\mu_\delta) + \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{d^n a(\mu)}{(d \ln \mu^2)^n} \right|_{\mu=\mu_\delta} (-\delta)^n, \quad (3)$$

where we used $\ln \mu_0^2 / \mu_\delta^2 = -\delta$. Then ρ in \mathcal{R}_δ to order a^4 reads:

$$\begin{aligned} \rho_\delta(Q^2) = & r_0 + r_1 a_1(\mu_1) + (r_2 + \beta_0 r_1 \delta_1) a_2(\mu_2)^2 \\ & + [r_3 + \beta_1 r_1 \delta_1 + 2\beta_0 r_2 \delta_2 + \beta_0^2 r_1 \delta_1^2] a_3(\mu_3)^3 \\ & + [r_4 + \beta_2 r_1 \delta_1 + 2\beta_1 r_2 \delta_2 + 3\beta_0 r_3 \delta_3 + 3\beta_0^2 r_2 \delta_2^2 \\ & + \beta_0^3 r_1 \delta_1^3 + \frac{5}{2} \beta_1 \beta_0 r_1 \delta_1^2] a_4(\mu_4)^4 + \mathcal{O}(a^5), \quad (4) \end{aligned}$$

where $\mu_i^2 = Q^2 e^{\delta_i}$, the initial scale is for simplicity set to $\mu_0^2 = Q^2$, and we defined $r_i(1) = r_i$. An artificial index was introduced on each a and δ to keep track of which coupling each δ term is associated with. The initial scale choice is arbitrary and is not the final argument of the running coupling; the final scales will be independent of the initial renormalization scale.

In a conformal (or scale-invariant) theory, where $\{\beta_i\} = \{0\}$, the δ dependence vanishes in Eq. (4). Therefore, by absorbing all $\{\beta_i\}$ dependence into the running coupling at each order, we obtain a final result independent of the initial choice of scale and scheme. The use of \mathcal{R}_δ allows us to put this on rigorous grounds. From the explicit expression in Eq. (4), it is easy to confirm that

$$\frac{\partial \rho_\delta}{\partial \delta} = -\beta(a) \frac{\partial \rho_\delta}{\partial a}. \quad (5)$$

The scheme invariance of the physical prediction requires that $\partial \rho_\delta / \partial \delta = 0$. Therefore, the scales in the running coupling must be shifted and set such that the conformal terms associated with the β function are removed; the remaining conformal terms are by definition renormalization scheme independent. The numerical value for the prediction at finite order is then scheme independent as required by the renormalization group. The scheme-invariance criterion is a theoretical requirement of the renormalization group; it must be satisfied at any truncated order of the perturbative series, and it is different from the formal statement that the all-orders expression for a physical observable is renormalization-scale

and scheme invariant; i.e., $d\rho/d\mu_0 = 0$. The final series obtained corresponds to the theory for which $\beta(a) = 0$, i.e., the conformal series. This demonstrates to any order the concept of the principal of maximum conformality (PMC) [3,4], which states that all nonconformal terms in the perturbative series must be resummed into the running coupling.

The expression in Eq. (4) exposes the pattern of $\{\beta_i\}$ terms in the coefficients at each order. Such a pattern was recently considered in Ref. [5]. The \mathcal{R}_δ scheme reveals its origin and its generality for any pQCD prediction. It is possible to infer more from Eq. (4): since there is nothing special about a particular value of δ , we conclude that some of the coefficients of the $\{\beta_i\}$ terms are degenerate; e.g., the coefficient of $\beta_0 a(Q)^2$ and $\beta_1 a(Q)^3$ can be set equal. Thus, for any scheme, the expression for ρ can be put to the form:

$$\begin{aligned} \rho(Q^2) = & r_{0,0} + r_{1,0} a(Q) + [r_{2,0} + \beta_0 r_{2,1}] a(Q)^2 \\ & + [r_{3,0} + \beta_1 r_{2,1} + 2\beta_0 r_{3,1} + \beta_0^2 r_{3,2}] a(Q)^3 \\ & + [r_{4,0} + \beta_2 r_{2,1} + 2\beta_1 r_{3,1} + \frac{5}{2} \beta_1 \beta_0 r_{3,2} \\ & + 3\beta_0 r_{4,1} + 3\beta_0^2 r_{4,2} + \beta_0^3 r_{4,3}] a(Q)^4 + \mathcal{O}(a^5), \quad (6) \end{aligned}$$

where the $r_{i,0}$ are the conformal parts of the perturbative coefficients; i.e., $r_i = r_{i,0} + \mathcal{O}(\{\beta_i\})$. The \mathcal{R}_δ scheme not only illuminates the $\{\beta_i\}$ pattern, but it also exposes a special degeneracy of coefficients at different orders. The degenerate coefficients can themselves be functions of $\{\beta_i\}$; hence, Eq. (6) is not to be understood as an expansion in $\{\beta_i\}$, but a pattern in $\{\beta_i\}$ with degenerate coefficients that must be matched. We have checked that this degeneracy holds for several known results.

The expansion in Eq. (4) reveals how the $\{\beta_i\}$ terms must be absorbed into the running coupling. The different δ_k 's keep track of the power of the $1/\epsilon$ divergence of the associated diagram at each loop order in the following way: the $\delta_k^p a^n$ term indicates the term associated with a diagram with $1/\epsilon^{n-k}$ divergence for any p . Grouping the different δ_k terms, one recovers in the $N_c \rightarrow 0$ Abelian limit [6] the dressed skeleton expansion. Resumming the series according to this expansion thus correctly reproduces the QED limit of the observable and matches the conformal series with running coupling constants evaluated at effective scales at each order.

Using this information from the δ_k expansion, it can be shown that the order $a(Q)^k$ coupling must be resummed into the effective coupling $a(Q_k)^k$, given by

$$r_{1,0} a(Q_1) = r_{1,0} a(Q) - \beta(a) r_{2,1} + \frac{1}{2} \beta(a) \frac{\partial \beta}{\partial a} r_{3,2} + \cdots + \frac{(-1)^n}{n!} \frac{d^{n-1} \beta}{(d \ln \mu^2)^{n-1}} r_{n+1,n}, \quad (7)$$

⋮

$$r_{k,0} a(Q_k)^k = r_{k,0} a(Q)^k + r_{k,0} k a(Q)^{k-1} \beta(a) \{R_{k,1} + \Delta_k^{(1)}(a) R_{k,2} + \cdots + \Delta_k^{(n-1)}(a) R_{k,n}\}, \quad (8)$$

which defines the PMC scales Q_k and where we introduced

$$R_{k,j} = (-1)^j \frac{r_{k+j,j}}{r_{k,0}}, \quad \Delta_k^{(1)}(a) = \frac{1}{2} \left[\frac{\partial \beta}{\partial a} + (k-1) \frac{\beta}{a} \right], \dots \quad (9)$$

Equation (8) is systematically derived by replacing the $\ln^j Q_1^2/Q^2$ by $R_{k,j}$ in the logarithmic expansion of $a(Q_k)^k$ up to the highest known $R_{k,n}$ coefficient in pQCD. The resummation can be performed iteratively using the renormalization group equation for a and leads to the effective scales for a next-to-next-to-next-to leading order (NNNLO) prediction (detailed derivations will be given elsewhere [2]):

$$\ln \frac{Q_k^2}{Q^2} = \frac{R_{k,1} + \Delta_k^{(1)}(a)R_{k,2} + \Delta_k^{(2)}(a)R_{k,3}}{1 + \Delta_k^{(1)}(a)R_{k,1} + [\Delta_k^{(1)}(a)]^2(R_{k,2} - R_{k,1}^2) + \Delta_k^{(2)}(a)R_{k,1}^2}. \quad (10)$$

The final pQCD prediction for ρ after setting the PMC scales Q_i then reads

$$\rho(Q^2) = r_{0,0} + r_{1,0}a(Q_1) + r_{2,0}a(Q_2)^2 + r_{3,0}a(Q_3)^3 + r_{4,0}a(Q_4)^4 + \mathcal{O}(a^5), \quad (11)$$

Note that Q_4 remains unknown. This last ambiguity resides only in the highest order coupling constant, and is negligible in practice.

It is easy to see to leading logarithmic order (LLO) that the effective scales are independent of the initial renormalization scale μ_0 . This follows since taking $\mu_0 \neq Q$ we must replace $R_{k,1} \rightarrow R_{k,1} + \ln Q^2/\mu_0^2$ and thus the leading order effective scales read $\ln Q_{k,\text{LO}}^2/\mu_0^2 = R_{k,1} + \ln Q^2/\mu_0^2$, where μ_0 cancels and Eq. (10) at leading logarithmic order is recovered. This generalizes to any order. In practice, however, since the β function is not known to all orders, a higher order residual renormalization-scale dependence will enter through the running coupling constant. This residual renormalization-scale dependence is strongly suppressed in the perturbative regime of the coupling [7].

The effective scales contain all the information of the nonconformal parts of the initial pQCD expression for ρ in Eq. (6), which is exactly the purpose of the running coupling constant. The quotient form of Eq. (10) sums up an infinite set of terms related to the known $r_{j,k \neq 0}$ which appear at every higher order due to the special degeneracy. It is, however, not the full solution since this requires the knowledge of the $r_{j,k \neq 0}$ terms to all orders. The method systematically sums up all known nonconformal terms, in principle to all orders, but is in practice truncated due to the limited knowledge of the β function.

In earlier PMC scale setting [4], and its predecessor, the Brodsky-Lepage-Mackenzie (BLM) method [8], the PMC/BLM scales have been set by using a perturbative expansion in a and only approximate conformal series have been obtained. Here, we have been able to obtain the conformal series exactly due to the revelation of the $\{\beta_i\}$ pattern by \mathcal{R}_δ ; the effective scales have naturally become functions of the coupling constant through the β function, in principle, to all orders.

In many cases the coefficients in a pQCD expression for an observable are computed numerically, and the $\{\beta_i\}$

dependence is not known explicitly. It is, however, easy to extract the dependence on the number of quark flavors N_f , since N_f enters analytically in any loop diagram computation. To use the systematic method presented in this Letter one puts the pQCD expression into the form of Eq. (6). Because of the special degeneracy in the coefficient of the $\{\beta_i\}$ terms, the N_f series can be matched to the $r_{j,k}$ coefficients in a unique way. (In principle, one must treat the N_f terms unrelated to renormalization of the gauge coupling as part of the conformal coefficient.) This allows one to automate the scale setting process algorithmically.

The general N_f series of the n th order coefficient in pQCD reads:

$$r_n = c_{n,0} + c_{n,1}N_f + \dots + c_{n,n-1}N_f^{n-1}. \quad (12)$$

By inspection of Eq. (6) it is seen that there are exactly as many unknown coefficients in the $\{\beta_i\}$ expansion at the order a^n as the N_f coefficients, $c_{n,j}$. This is realized due to the special degeneracy found in (6). The $r_{i,j}$ coefficients in Eq. (6) can thus be expressed in terms of the $c_{n,j}$ coefficients. This means that the N_f terms can unambiguously be associated with $\{\beta_i\}$ terms and demonstrates PMC as the underlying principle of BLM scale setting. The relations between $c_{n,j}$ and $r_{i,j}$ are easy to derive and they transform the BLM scales into the correct PMC scales [2].

The automation process can be outlined as follows. (i) Choose any δ -Renormalization scheme and scale, (ii) compute the physical observable in pQCD and extract the N_f coefficients, $c_{k,j}$, (iii) find the β_i coefficients, $r_{k,j}$ from the $c_{k,j}$ coefficients and compute the PMC scales, Q_k , (iv) the final pQCD expression for the observable reads $\rho_{\text{final}}(Q) = \sum_{k=0} r_{k,0} a(Q_k)^k$.

As a final remark, we note that the PMC can be used to set separate scales for different skeleton diagrams; this is particularly important for multiscale processes. In general, the $\{\beta_i\}$ coefficients multiply terms involving logarithms in each of the invariants [3]. For instance, in the case of $q\bar{q} \rightarrow Q\bar{Q}$ near the heavy quark threshold in pQCD, the PMC assigns different scales to the annihilation process and the rescattering corrections involving the heavy quarks' relative velocity [9]. It also can be used to set the scale for the "lensing" gluon-exchange corrections that

appear in the Sivers, Collins, and Boer-Mulders effects. Moreover, for the cases when the process involves several energy regions, e.g., hard, soft, etc., one may adopt methods such as the nonrelativistic QCD effective theory [10] and the soft-collinear effective theory [11] to set the PMC scales; i.e., one first sets the PMC scales for the higher energy region, then integrates it out to form a lower energy effective theory and sets the PMC scales for this softer energy region, etc. In this way one obtains different effective PMC scales for each energy region, at which all the PMC properties also apply.

Example: $e^+e^- \rightarrow \text{hadrons}$.—The ratio for electron-positron annihilation into hadrons, $R^{e^+e^- \rightarrow \text{h}}$, was recently computed to order a^4 [12] and can be shown to exactly match the generic form of Eq. (6). It can be derived by analytically continuing the Adler function D into the timelike region, with D given by

$$D(Q^2) = \gamma(a) - \beta(a) \frac{d}{da} \Pi(Q^2, a), \quad (13)$$

where γ is the anomalous dimension of the vector field, Π is the vacuum polarization function, and they are given by the perturbative expansions $\gamma(a) = \sum_{n=0}^{\infty} \gamma_n a^n$ and $\Pi(a) = \sum_{n=0}^{\infty} \Pi_n a^n$. It is easy to show that to order a^4 the perturbative expression for $R^{e^+e^- \rightarrow \text{h}}$ in terms of γ_n and Π_n reads:

$$\begin{aligned} R^{e^+e^- \rightarrow \text{h}}(Q) &= \gamma_0 + \gamma_1 a(Q) + [\gamma_2 + \beta_0 \Pi_1] a(Q)^2 \\ &+ \left[\gamma_3 + \beta_1 \Pi_1 + 2\beta_0 \Pi_2 \right. \\ &- \left. \beta_0^2 \frac{\pi^2 \gamma_1}{3} \right] a(Q)^3 + \left[\gamma_4 + \beta_2 \Pi_1 + 2\beta_1 \Pi_2 \right. \\ &+ 3\beta_0 \Pi_3 - \frac{5}{2} \beta_0 \beta_1 \frac{\pi^2 \gamma_1}{3} \\ &- \left. 3\beta_0^2 \frac{\pi^2 \gamma_2}{3} - \beta_0^3 \pi^2 \Pi_1 \right] a(Q)^4. \quad (14) \end{aligned}$$

This expression has exactly the form of Eq. (6) with the identification $r_{i,0} = \gamma_i$, $r_{i,1} = \Pi_{i-1}$, $r_{i,2} = -(\pi^2/3)\gamma_{i-2}$, and $r_{i,3} = -\pi^2 \Pi_{i-3}$. The γ_i contain N_f terms, but since they are independent of δ to any order, they are kept fixed in the scale-setting procedure. Note that we have knowledge of even higher order $r_{i,j}$ coefficients, and this allows us to set the effective scales Q_1 , Q_2 , and Q_3 to the NNNLO, given by Eq. (10). It is worth noting that the Adler function D itself has a much simpler $\{\beta_i\}$ structure. By convention, the argument of a is spacelike; thus, the π^2 terms appearing in $R^{e^+e^- \rightarrow \text{h}}$ could be avoided by using a coupling constant with a timelike argument, leading to a more convergent series [13].

The last unknown scale in Eq. (14) can be estimated. It turns out that $Q_4 \sim Q$, which is the value we have used [2]. The expressions for the coefficients γ_i and Π_i can be found

in Ref. [12], and the four-loops β function is given in Ref. [14]. The final result in numerical form in terms of $\alpha = \alpha_s/\pi$ for QCD with five active flavors reads:

$$\begin{aligned} \frac{3}{11} R^{e^+e^- \rightarrow \text{h}}(Q) &= 1 + \alpha(Q_1) + 1.84\alpha(Q_2)^2 \\ &- 1.00\alpha(Q_3)^3 - 11.31\alpha(Q_4)^4. \quad (15) \end{aligned}$$

This is a more convergent result compared to previous estimates, and it is free of any scheme and scale ambiguities (up to strongly suppressed residual ones).

To find numerical values for the effective scales, the asymptotic scale Λ of the running coupling must first be determined by matching Eq. (15) with experimental results [15]: $\frac{3}{11} R_{\text{exp}}^{e^+e^- \rightarrow \text{h}}(\sqrt{s} = 31.6 \text{ GeV}) = 1.0527 \pm 0.0050$. Using a logarithmic expansion solution of the renormalization group equation for a we find $\Lambda_{\overline{\text{MS}}} = 419_{-168}^{+222} \text{ MeV}$. We have used the $\overline{\text{MS}}$ definition for the asymptotic scale, and the asymptotic scale of \mathcal{R}_δ can be taken to be the same for any δ . The effective scales are found to be $Q_1 = 1.3Q$, $Q_2 = 1.2Q$, $Q_3 \approx 5.3Q$. The values are independent of the initial renormalization scale up to some residual dependence coming from the truncated β function, which is less than the quoted accuracy on the numbers. This is illustrated in Fig. 1. For Q_3 we have taken the LO value, which is sufficient to get the conformal series at four loops. Its higher order value has artificial strong residual renormalization-scale dependence due to the large numerical value of Π_3 in QCD with five active flavors. These final scales determine the effective number of quark flavors at each order of perturbation theory [16].

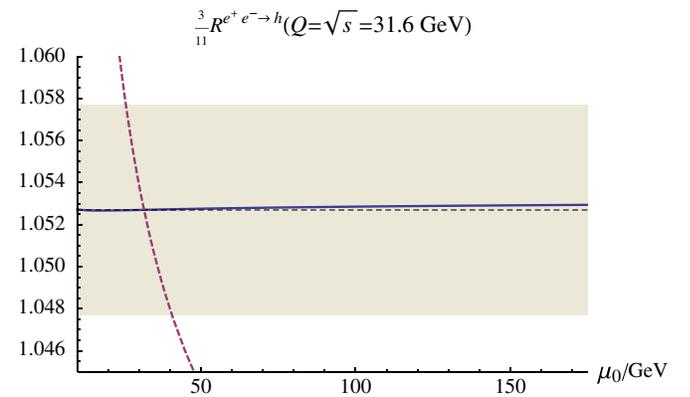


FIG. 1 (color online). The final PMC result for $R^{e^+e^- \rightarrow \text{h}}$ as a function of the initial renormalization scale μ_0 (solid blue line), demonstrating the initial scale invariance of the final prediction, up to strongly suppressed residual dependence. The shaded region is the experimental bounds with the central value given by the thin dashed line. For comparison we also show the pQCD prediction before PMC scale setting (thick dashed red line) fixed to the experimental value for $\mu_0 = Q$. The result is very sensitive to μ_0 , and thus it severely violates renormalization group properties.

For completeness, we use our final result to predict the strong coupling constant at the Z -boson mass scale in five flavor massless QCD:

$$\alpha_s(M_Z) = 0.132_{-0.011}^{+0.010}. \quad (16)$$

The error on this result is a reflection of the experimental uncertainty on $R_{\text{exp}}^{e^+e^- \rightarrow h}$, which cannot be eliminated. This value is somewhat larger than the present world average $\alpha_s(M_Z) = 0.1184 \pm 0.0007$, which is a global fit of all types of experiments. However, it is consistent with the values obtained from e^+e^- colliders, i.e., $\alpha_s(M_Z) = 0.13 \pm 0.005 \pm 0.03$ by the CLEO Collaboration [17] and $\alpha_s(M_Z) = 0.1224 \pm 0.0039$ from the jet shape analysis [18]. Moreover, in computing $\alpha_s(M_Z)$ we have assumed massless quarks. The estimate will decrease when taking threshold effects properly into account as shown in [19].

We can apply our result to Abelian QED, where $R^{e^+e^- \rightarrow h}$ can be seen as the imaginary part of the QED four loop 1PI vacuum polarization diagram by the optical theorem, and find in this case nearly complete renormalization-scale independence of all three scales to the NNNLO due to the small value of the coupling constant. Numerically, we get for three (lepton) flavors:

$$\frac{1}{3} R_{\text{QED}}^{e^+e^- \rightarrow \ell}(Q) = 1 + 0.24\alpha_e(Q_1) - 0.08\alpha_e(Q_2)^2 - 0.13\alpha_e(Q_3)^3 + 0.05\alpha_e(Q_4)^4, \quad (17)$$

where $\alpha_e = e^2/4\pi$ and $\{Q_1, Q_2, Q_3\} = \{1.1, 0.6, 0.5\}$.

In this Letter we have shown that a generalization of the conventional $\overline{\text{MS}}$ scheme is illuminating. It enables one to determine the general (and degenerate) pattern of non-conformal $\{\beta_i\}$ terms and to systematically determine the argument of the running coupling order by order in pQCD, in a way which is readily automatized. The resummed series matches the conformal series, in which no factorially divergent $n!\beta^n\alpha_s^n$ “renormalon” series appear and which is free of any scheme and scale ambiguities. This is the final expression one should use for physical predictions. The method can be applied to processes with multiple physical scales and is consistent with QED scale setting in the limit $N_C \rightarrow 0$. The new method satisfies all of the principles of the renormalization group, including the principle of maximum conformality, and it eliminates an unnecessary source of systematic error.

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*mojaza@slac.stanford.edu

†sjbth@slac.stanford.edu

‡wuxg@cqu.edu.cn

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