SLAC-PUB-14774

Scale Setting Using the Extended Renormalization Group and the Principle of Maximum Conformality: the QCD Coupling Constant at Four Loops

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(Dated: December 2, 2011)

A key problem in making precise perturbative QCD predictions is to set the proper renormalization scale of the running coupling. The extended renormalization group equations, which express the invariance of physical observables under both the renormalization scale- and scheme-parameter transformations, provide a convenient way for estimating the scale- and scheme-dependence of the physical process. In this paper, we present a solution for the scale-equation of the extended renormalization group equations at the four-loop level. Using the principle of maximum conformality (PMC) / Brodsky-Lepage-Mackenzie (BLM) scale-setting method, all non-conformal $\{\beta_i\}$ terms in the perturbative expansion series can be summed into the running coupling, and the resulting scale-fixed predictions are independent of the renormalization scheme. Different schemes lead to different effective PMC/BLM scales, but the final results are scheme independent. Conversely, from the requirement of scheme independence, one not only can obtain scheme-independent commensurate scale relations among different observables, but also determine the scale displacements among the PMC/BLM scales which are derived under different schemes. In principle, the PMC/BLM scales can be fixed order-by-order, and as a useful reference, we present a systematic and scheme-independent procedure for setting PMC/BLM scales up to NNLO. An explicit application for determining the scale setting of $R_{e^+e^-}(Q)$ up to four loops is presented. By using the world average $\alpha_s^{\overline{MS}}(M_Z) = 0.1184 \pm 0.0007$, we obtain the asymptotic scale for the 't Hooft associated with the $\overline{MS}$ scheme, $\Lambda_{\overline{MS}}^{'tH} = 245^{+9}_{-10}$ MeV, and the asymptotic scale for the conventional $\overline{MS}$ scheme, $\Lambda_{\overline{MS}} = 213^{+19}_{-8}$ MeV.

PACS numbers: 12.38.Aw, 11.10.GH, 11.15.Bt

I. INTRODUCTION

All physical predictions in QCD should in principle be invariant under any choice of renormalization scale and scheme. However at any finite order, the use of different scales and schemes may lead to different theoretical predictions. The optimal procedure for obtaining precise QCD predictions is to choose the renormalization scale so that the result is scheme independent at any fixed order of α_s. Moreover, the result for a scale-setting strategy should satisfy several self-consistent conditions: the existence and uniqueness of the scale, reflexivity, symmetry and transitivity [1]. Perturbative QCD becomes an Abelian theory at $N_c \to 0$, so QCD scale setting must also agree with that of QED in this limit [2]. We shall show that the Brodsky-Lepage-Mackenzie method (BLM) [3] and the Principle of Maximum Conformality (PMC) [4] provide a solution to this problem [1].

The main idea of PMC/BLM is that after proper procedures, all non-conformal $\{\beta_i\}$ terms in the perturbative expansion are summed into the running coupling and the remaining terms in the perturbative series are identical to that of a conformal theory, i.e. the corresponding theory with $\{\beta_i\} = \{0\}$. The QCD predictions from PMC/BLM are then independent of renormalization scheme. It has been found that PMC/BLM satisfies all self-consistent conditions [1]. After PMC/BLM scale setting, the divergent "renormalon" series of order $(n!\beta_i^n\alpha_s^n)$ does not appear in the conformal series; thus as in QED, the scale can be unambiguously set by PMC/BLM.

One can use PMC/BLM method to relate perturbative calculable observables in QCD, i.e. to derive commensurate scale relations among different observables, whose coefficients can be identified with those obtained in conformally invariant gauge theory exactly [5, 6]. Moreover, from the requirement of scheme-independence, one can determine the displacements among the PMC/BLM scales that are derived under different schemes or conventions. We shall show how to fix the PMC/BLM scales order-by-order. One way to set the leading order (LO) and the next-to-leading order (NLO) PMC/BLM scales has been suggested in the literature [3–5]. Concerning the recent improvements on perturbative QCD calculations and the need to improve the theoretical predictions to confront more and more accurate experimental data, it shall be interesting to provide a systematic and scheme-independent treatment of PMC/BLM up to next-to-next-to-leading order (NNLO).

As an extension to the conventional renormalization group (RG) equation, the extended RG equations express the invariance of physical observables under both

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[1] PMC provides the principle underlying BLM scale setting, so if not specially stated, we usually treat them on equal footing.

Work supported in part by US Department of Energy contract DE-AC02-76SF00515.

the renormalization scale- and scheme-parameter transformations [7, 8]. In this approach, a universal coupling function which covers all possible choices of scale and scheme is introduced, whose corresponding perturbative series serves as an intermediate device for the identification of scale and scheme parameters. It can be treated as a transparent solution to the scale-scheme ambiguity problem. A useful advantage is that the scheme dependence can be reliably estimated through the scheme equations. This approach also provides a platform for a reliable scheme-error analysis and a precise definition for the asymptotic scale under a possible renormalization scheme R, i.e. the scale for the 't Hooft associated with R-scheme $\Lambda_R^{'tH}$ [8]. We shall present a general solution for the extended RG equation and give some relations between the universal coupling function and the conventional adopted coupling function.

The remaining parts of the paper are organized as follows: in Sec.II, we give the extended RG equations and provide its solution up to four loops. In Sec.III, we present a systematic procedure for setting PMC/BLM scales up to NNLO. Discussions and an explicit application are also presented in Sec.III. Sec.IV provides a summary.

II. EXTENDED RENORMALIZATION GROUP EQUATIONS

Under an arbitrary renormalization scheme, hereafter refers to as R-scheme, the scale dependence of the coupling constant is controlled by the RG equation

$$\frac{d}{d\ln\mu^2}\left(\frac{\alpha_s^R(\mu)}{4\pi}\right) = -\sum_{i=0}^{\infty}\beta_i^R\left(\frac{\alpha_s^R(\mu)}{4\pi}\right)^{i+2}. \quad (1)$$

Various terms in β_0, β_1, $\cdots$, correspond to one loop, two loop $\cdots$ contributions respectively. Generally $\{\beta_i\}$ depend on quark mass m_f through the variable m_f^2/μ^2. According to the decoupling theorem, quark with mass $m_f \gg \mu$ can be ignored, and we can often neglect m_f-terms when $m_f \ll \mu$. Then, for every μ we divide the quarks into active ones with $m_f = 0$ and the inactive ones that can be simply ignored. Within this framework, it is well-known that the first two coefficients β_0 and β_1 are universal, while all higher-order coefficients $\{\beta_i^R\}_{i\geq 2}$ are renormalization scheme dependent. Under the $\overline{MS}$ scheme, $\{\beta_i\}$ up to four loops can be found in the literature [9].

With the help of the two universal coefficients β_0 and β_1, one can change the RG equation into a simpler canonical form by rescaling the coupling constant as $a^R = \beta_1\alpha_s^R/(4\pi\beta_0)$ and the scale parameter as $\tau = (\beta_0^2/\beta_1)\ln\mu^2$, i.e.

$$\frac{da^R}{d\tau} = -(a^R)^2\left[1 + a^R + c_2^R(a^R)^2 + c_3^R(a^R)^3 + \cdots\right], \quad (2)$$

where $c_i^R = \beta_i^R\beta_0^{i-1}/\beta_1^i$. Furthermore, one can define a universal coupling constant $a(\tau,\{c_i\})$ to include the dependence on the scheme parameters $\{c_i\}$, which satisfies the following extended RG equations [7, 8]

$$\beta(a,\{c_i\}) = \frac{\partial a}{\partial\tau} = -a^2\left[1 + a + c_2a^2 + c_3a^3 + \cdots\right] \quad (3)$$

and

$$\beta_n(a,\{c_i\}) = \frac{\partial a}{\partial c_n} = -\beta(a,\{c_i\})\int_0^a \frac{x^{n+2}dx}{\beta^2(x,\{c_i\})} \quad (4)$$

The scale-equation (3), similar to Eq.(2), can be used to evolve the coupling function from one scale to another. By comparing Eq.(2) with Eq.(3), there exists a value of $\tau = \tau_R$ for which,

$$a^R(\tau_R) = a(\tau_R,\{c_i^R\}). \quad (5)$$

This shows that any coupling constant $a^R(\tau)$ can be expressed by a universal coupling constant $a(\tau,\{c_i\})$ under proper correspondence. The scheme-equation (4) can be used to relate the coupling functions under different schemes by changing $\{c_i\}$. It is noted that the universal coupling function has a particularly simple form when all the scheme parameters $\{c_i\}$ are set to zero, i.e. the coupling function can be written as a function of the scale in terms of the Lambert W function [10]. Such a special case with $\{c_i\} \equiv \{0\}$ is usually called as the 't Hooft scheme [11]. In addition to simplifying the solution of the RG equations, the 't Hooft scheme also provides a precise definition for the asymptotic scale Λ of QCD as will be shown below [2].

Integrating Eq.(3) leads to

$$L = \mathcal{C} + \frac{1}{a} + \ln a + (c_2 - 1)\,a + \frac{c_3 - 2c_2 + 1}{2}a^2 + \mathcal{O}(a^3), \quad (6)$$

where $L = (\beta_0^2/\beta_1)\ln(\mu^2/\Lambda^2)$ and Λ is the asymptotic scale parameter. The integration constant $\mathcal{C}$ is arbitrary, whose value depends on how we set the asymptotic scale Λ. Since the 't Hooft scheme is free of high-order corrections, it provides a precise definition for Λ, i.e. the 't Hooft scale $\Lambda^{'tH}$, which is defined to be the pole of the coupling function in the 't Hooft scheme, $a^{'tH} \equiv a(2\beta_0^2/\beta_1\ln(\mu/\Lambda^{'tH}),\{0\})$. $\Lambda^{'tH}$ is not unique, and there are infinite number of 't Hooft schemes, differing only by the value of $\Lambda^{'tH}$. However under a specific renormalization scheme (R-scheme), its asymptotic scale can be fixed to be the 't Hooft scale associated with the R-scheme $\Lambda_R^{'tH}$ [8], which enters into both $a^R(\mu) = a(2\beta_0^2/\beta_1\ln(\mu/\Lambda_R^{'tH}),\{c_i^R\})$ and $a^{'tH-R}(\mu) =$

[2] Recently, it has been found that the 't Hooft scheme fails to reproduce the factorized form of the $\overline{MS}$-scheme generalization of the generalized Crewther relation [12]. This shows that one cannot use it for studying special theoretical features of gauge theories beyond the two-loop level.

$a(2\beta_0^2/\beta_1 \ln(\mu/\Lambda_R^{\prime tH}), \{0\})$. Here the word "associated" means we are choosing the particular 't Hooft scheme that shares the same 't Hooft scale with the R-scheme.

Eq.(6) can be solved iteratively, and its solution can be expanded as a power series of $1/L$, i.e. up to four loops,

$$a = \frac{1}{L} + \frac{1}{L^2}\left(\mathcal{C} - \ln L\right) + \frac{1}{L^3}\left[\mathcal{C}^2 + \mathcal{C} + c_2 - (2\mathcal{C} - \ln L + 1)\ln L - 1\right] + \frac{1}{L^4}\left\{\mathcal{C}\left(\mathcal{C}^2 + \frac{5}{2}\mathcal{C} + 3c_2 - 2\right) - \frac{1-c_3}{2} - \left[3\mathcal{C}^2 + 5\mathcal{C} + 3c_2 - 2 - \left(3\mathcal{C} - \ln L + \frac{5}{2}\right)\ln L\right]\ln L\right\} + \mathcal{O}\left(\frac{1}{L^5}\right). \quad (7)$$

As a cross-check, the above solution agrees with Ref.[13] after proper parameter transformations and by identifying the integration constant $\mathcal{C}^*$ used there to be $\mathcal{C}^* = \frac{\beta_1}{\beta_0^2}\left(\mathcal{C} - \ln\frac{4\beta_0}{\beta_1}\right)$. When setting $\{c_i\} = \{0\}$ and $\mathcal{C} = 0$, we recover the coupling constant under the 't Hooft scheme. One can also obtain a relation between $\Lambda_R^{\prime tH}$ and Λ_R, i.e.

$$\Lambda_R^{\prime tH} = \exp\left(\frac{\beta_1}{2\beta_0^2}\mathcal{C}_R\right)\Lambda_R. \quad (8)$$

As a special case, by choosing $\mathcal{C}_{\overline{MS}} = \ln\beta_0^2/\beta_1$, we obtain

$$\Lambda_{\overline{MS}}^{\prime tH} = \left(\frac{\beta_1}{\beta_0^2}\right)^{-\beta_1/2\beta_0^2}\Lambda_{\overline{MS}}, \quad (9)$$

which agrees with the observation in Ref.[8]. The present definition of $\Lambda_{\overline{MS}}$ is the conventional one suggested by Ref.[14, 15]; there are other choices for $\mathcal{C}_{\overline{MS}}$ [16], which might be helpful in certain cases.

III. BLM SCALE SETTING UP TO NNLO

Generally, perturbative QCD prediction for a physical observable ρ can be written as

$$\rho = r_0\Big[a_s^n(Q) + (A_1 + A_2 n_f)a_s^{n+1}(Q) + (B_1 + B_2 n_f + B_3 n_f^2)a_s^{n+2}(Q) + (C_1 + C_2 n_f + C_3 n_f^2 + C_4 n_f^3)a_s^{n+3}(Q) + \cdots\Big] \quad (10)$$

where $a_s(Q) = \left(\frac{\alpha_s(Q)}{\pi}\right)$ and the overall tree-level parameter r_0 is scale-independent and is free of $a_s(Q)$. Here n_f stands for the quark flavor number and $n(\geq 1)$ stands for the initial α_s order at the tree level. After proper scale setting, all n_f-terms in the perturbative expansion can be summed into the running coupling. Here, we shall concentrate on those processes in which all n_f-terms are associated with the $\{\beta_i\}$-terms. In higher-order processes, there may be n_f-terms coming from the light-by-light quark loops which are irrelevant to the ultra-violet cutoff; they have no relation to the $\{\beta_i\}$-terms [3]. Those terms should be identified and kept separately after the BLM scale setting [3].

The BLM scales can be set up in a general scheme-independent way, and the generalization of the BLM procedure to higher order assigns a different renormalization scale for each other in the perturbative series, which can be done order by order. We can shift the renormalization scale Q into effective ones until we fully absorb those higher-order terms with n_f-dependence into the running coupling [4].

More explicitly, the first step of the BLM method is to set the effective scale Q^* at LO

$$\rho = r_0\Big[a_s^n(Q^*) + \widetilde{A}_1 a_s^{n+1}(Q^*) + (\widetilde{B}_1 + \widetilde{B}_2 n_f)a_s^{n+2}(Q^*) + (\widetilde{C}_1 + \widetilde{C}_2 n_f + \widetilde{C}_3 n_f^2)a_s^{n+3}(Q^*) + \cdots\Big]. \quad (11)$$

The second step is to set the effective scale Q^{**} at NLO

$$\rho = r_0\Big[a_s^n(Q^*) + \widetilde{A}_1 a_s^{n+1}(Q^{**}) + \widetilde{\widetilde{B}}_1 a_s^{n+2}(Q^{**}) + (\widetilde{\widetilde{C}}_1 + \widetilde{\widetilde{C}}_2 n_f)a_s^{n+3}(Q^{**}) + \cdots\Big], \quad (12)$$

and the final step is to set the effective scale Q^{***} at NNLO

$$\rho = r_0\Big[a_s^n(Q^*) + \widetilde{A}_1 a_s^{n+1}(Q^{**}) + \widetilde{\widetilde{B}}_1 a_s^{n+2}(Q^{***}) + \widetilde{\widetilde{\widetilde{C}}}_1 a_s^{n+3}(Q^{***}) + \cdots\Big]. \quad (13)$$

When performing the scale shifts $Q \to Q^*$, $Q^* \to Q^{**}$ and $Q^{**} \to Q^{***}$, we eliminate the n_f-terms associated with the $\{\beta_i\}$-terms completely, but at the same time we also have to modify the coefficients. To set the effective scale for a_s^{n+3}, one needs even higher order information and here, a sensible choice is Q^{***}, since this is the renormalization scale after shifting the scales in the final step of the BLM procedure up to NNLO. Note that the effective scales should be a perturbative series of a_s so as

[3] Those n_f-terms, coming from the light-quark loops connected to at least four photon/gluon lines, are of higher twists and power suppressed by hard scales, so they usually can be safely neglected.

[4] Another way to set the BLM scale up to NNLO can be found in Refs.[17, 18], where a unified effective scale Q^* is used for all orders.

to absorb all n_f-dependent terms properly, and up to NNLO, three effective scales can be written as

$$\ln\frac{Q^{*2}}{Q^2}=\ln\frac{Q_0^{*2}}{Q^2}+\frac{x\beta_0}{4}\ln\frac{Q_0^{*2}}{Q^2}a_s(Q) +\frac{y}{16}\left(\beta_0^2\ln^2\frac{Q_0^{*2}}{Q^2}-\beta_1\ln\frac{Q_0^{*2}}{Q^2}\right)a_s^2(Q) \quad (14)$$

$$\ln\frac{Q^{**2}}{Q^{*2}}=\ln\frac{Q_0^{**2}}{Q^{*2}}+\frac{z\beta_0}{4}\ln\frac{Q_0^{**2}}{Q^{*2}}a_s(Q^*) \quad (15)$$

$$\ln\frac{Q^{***2}}{Q^{**2}}=\ln\frac{Q_0^{***2}}{Q^{**2}} \quad (16)$$

where the effective scales $Q_0^{*,**,***}$ are determined so as to eliminate A_2n_f, $\widetilde{B}_2n_f$ and $\widetilde{\widetilde{C}}_2n_f$-terms completely, the parameters x and z are used to eliminate the $B_3n_f^2$ and the $\widetilde{C}_3n_f^2$ terms respectively, and the parameter y is used to eliminate the $C_4n_f^3$-term. It is found that

$$\ln\frac{Q_0^{*2}}{Q^2}=\frac{6A_2}{n} \quad (17)$$

$$\ln\frac{Q_0^{**2}}{Q^{*2}}=\frac{6\widetilde{B}_2}{(n+1)\widetilde{A}_1} \quad (18)$$

$$\ln\frac{Q_0^{***2}}{Q^{**2}}=\frac{6\widetilde{\widetilde{C}}_2}{(n+2)\widetilde{\widetilde{B}}_1} \quad (19)$$

and

$$x=\frac{3(n+1)A_2^2-6nB_3}{nA_2} \quad (20)$$

$$y=\frac{(n+1)(2n+1)A_2^3-6n(n+1)A_2B_3+6n^2C_4}{nA_2^2} \quad (21)$$

$$z=\frac{3(n+2)\widetilde{B}_2^2-6(n+1)\widetilde{A}_1\widetilde{C}_3}{(n+1)\widetilde{A}_1\widetilde{B_2}} \quad (22)$$

The coefficients A_i, B_i, C_i and etc. are renormalization scheme dependent, so different renormalization schemes lead to different BLM scales $Q^{*,**,***}$; however the final result for ρ should be scheme independent. Using the argument, one can use BLM method to relate perturbative calculable observables, i.e. to derive commensurate scale relations among different observables. In fact, any perturbatively-calculable physical observable can be used to define an effective coupling constant by incorporating the entire radiative correction into its definition [20]; for example $R_{e^+e^-}(Q)\equiv R^0_{e^+e^-}(Q)\left[1+\frac{\alpha_s^R(Q)}{\pi}\right]$ defines an effective coupling constant $\alpha_s^R(Q)$, where $R^0_{e^+e^-}(Q)$ is the Born result. Any effective coupling constant can be used as a reference running coupling constant in QCD to define the renormalization procedure. More generally, each effective running coupling constant or renormalization scheme is a special case of the universal coupling function as shown by Eq.(5).

The NLO commensurate scale relations between different effective coupling constants can be found in Ref.[5]. Replacing the observable ρ by its corresponding effective coupling constant and changing a_s to be another effective coupling constant, starting form Eq.(10) and following the same procedures, one can naturally obtain the commensurate scale relations up to NNLO. Moreover, with the relations between $Q^{*,**,***}$ and Q, one can find the needed scale displacement among the effective scales that are derived under different schemes or conventions so as to ensure the scheme-independence of the observables. For example, from the relation between Q^* and Q, one can easily obtain the well-known one-loop relation for the coupling constant [3], $\alpha_s^{\overline{MS}}(e^{-5/3}Q^2)=\alpha_s^{GM-L}(Q^2)$, where the scale displacement $e^{-5/3}$ between the $\overline{MS}$ scheme and the Gell-Mann-Low scheme [21] is a result of the convention that is chosen to define the minimal dimensional regularization scheme [14].

The step-by-step coefficients which are introduced in Eqs.(11,12,13) are

$$\widetilde{A}_1=A_1+\frac{33}{2}A_2\ ,\ \widetilde{\widetilde{B}}_1=\widetilde{B}_1+\frac{33}{2}\widetilde{B}_2\ ,\ \widetilde{\widetilde{\widetilde{C}}}_1=\widetilde{\widetilde{C}}_1+\frac{33}{2}\widetilde{\widetilde{C}}_2 \quad (23)$$

$$\widetilde{B}_1=\frac{1}{4n}\left[1089(n+1)A_2^2+153nA_2+66(n+1)A_1A_2+(4B_1-1089B_3)n\right] \quad (24)$$

$$\widetilde{B}_2=\frac{-1}{4n}\left[66(n+1)A_2^2+19nA_2+4(n+1)A_1A_2-4n(B_2+33B_3)\right] \quad (25)$$

$$\widetilde{C}_1=\frac{1}{64A_2n^2}\Big[-40392C_4n^3+143748{A_2}^4(3+5n+2n^2)+8A_2n^2(8C_1+35937C_4+ 5049B_3n)-13464{A_2}^3n(n^2-3n-7)+72A_1A_2(1+n)(34A_2n-242B_3n+ 121{A_2}^2(3+2n))+3{A_2}^2n(2857n+352B_1(2+n)-95832B_3(3+2n))\Big] \quad (26)$$

$$\widetilde{C}_2=\frac{1}{192A_2n^2}\Bigg[22392C_4n^3-52272{A_2}^4(3+5n+2n^2)(3+2n)-24A_2n^2(-8C_2+6534C_4+933B_3n)-48A_1A_2(1+n)(19A_2n-132B_3n+66{A_2}^2(3+2n))+{A_2}^2n(-5033n-192B_1(2+n)+3168B_2(2+n)+52272B_3(8+5n))+24{A_2}^3n(-1871+n(-627+311n))\Bigg] \tag{27}$$

$$\widetilde{C}_3=\frac{1}{576A_2n^2}\Bigg[-2736C_4n^3+4752{A_2}^4(3+5n+2n^2)+144A_2n^2(4C_3+198C_4+19B_3n)-912{A_2}^3(n^3-4n)+288A_1A_2(1+n)(-2B_3n+{A_2}^2(3+2n))-{A_2}^2n(-325n+576B_2(2+n)+9504B_3(5+3n))\Bigg] \tag{28}$$

$$\widetilde{\widetilde{C}}_1=\frac{1}{4(n+1)\widetilde{A_1}}\Bigg[33(n+2)\widetilde{B_2}(2\widetilde{B_1}+33\widetilde{B_2})+(n+1)(153\widetilde{B_2}+4\widetilde{C_1}-1089\widetilde{C_3})\widetilde{A_1}\Bigg] \tag{29}$$

$$\widetilde{\widetilde{C}}_2=\frac{-1}{4(n+1)\widetilde{A_1}}\Bigg[2(n+2)\widetilde{B_2}(2\widetilde{B_1}+33\widetilde{B_2})+(n+1)(19\widetilde{B_2}-4(\widetilde{C_2}+33\widetilde{C_3}))\widetilde{A_1}\Bigg] \tag{30}$$

(31)

In deriving the above formulae, the following equation is implicitly adopted, i.e. the running of a_s at any scale Q^* can be obtained from its value at an initial scale Q,

$$a_s(Q^*)=a_s(Q)\left[1+\frac{\beta_0}{4}\ln\left(\frac{Q^{*2}}{Q^2}\right)a_s(Q)+\frac{\beta_1}{4^2}\ln\left(\frac{Q^{*2}}{Q^2}\right)a_s^2(Q)+\frac{\beta_2}{4^3}\ln\left(\frac{Q^{*2}}{Q^2}\right)a_s^3(Q)+\cdots\right]^{-1} \tag{32}$$

A. PMC and BLM correspondence principle

A systematic procedure for setting PMC scale at LO has been suggested in Ref.[4]. The main procedure is to distinguish the nonconformal terms from the conformal terms by the variation of the cross section with respect to $(\ln\mu_0^2)$ (μ_0 stands for some initial scale of the process). Since at LO, there is only one $\{\beta_i\}$-term (i.e. β_0) and the identified nonconformal terms always have the form $(\beta_0\ln\mu_0^2)$, one can determine the nonconformal terms exactly. However, at higher orders, the $\ln\mu_0^2$-terms are usually in power series as $\beta_0\ln\mu_0^2$, $\beta_1\ln\mu_0^2$, $\beta_0^2(\ln\mu_0^2)^2$ and etc.. So this method is no longer adaptable to deal with higher order corrections, because the derivative with respect to a single $\left(\ln\mu_0^2\right)$ cannot distinguish all the emerged $\{\beta_i\}$-terms. Some alternative should be introduced.

The purpose of the running coupling in any gauge theory is to sum up all the terms involving the $\{\beta_i\}$-functions, conversely, one can find all the needed $\{\beta_i\}$-terms at any concerned order from the expansion of the running coupling (32) [5]. Using this fact and also the relation between $\{\beta_i\}$ and n_f, one can obtain the PMC scales from the BLM scale-setting method up to NNLO. We call this the PMC and BLM correspondence principle. Note that $\{\beta_i\}$ $(i\geq 2)$ are scheme-dependent, so the PMC and BLM correspondence depends on the scheme beyond the two-loop level.

More explicitly, up to NNLO, the physical observable can be expanded in the $\{\beta_i\}$-series as,

$$\rho=r_0\Big[a_s^n(Q)+(A_1^0+A_2^0\beta_0)a_s^{n+1}(Q)+(B_1^0+B_2^0\beta_1+B_3^0\beta_0^2)a_s^{n+2}(Q)+(C_1^0+C_2^0\beta_2+C_3^0\beta_0\beta_1+C_4^0\beta_0^3)a_s^{n+3}(Q)\Big]. \tag{33}$$

The results for the PMC can be naturally obtained from the BLM scale setting through proper parameter corre-

[5] It is noted that such an expansion is different from that of Refs.[18, 19], where all the $\{\beta_i\}$-terms which may contribute at the same order have been introduced to deal with the Adler D-function.

spondence, i.e.

$$A_1 = A_1^0 + 11A_2^0 \tag{34}$$
$$A_2 = -\frac{2}{3}A_2^0 \tag{35}$$
$$B_1 = B_1^0 + 102B_2^0 + 121B_3^0 \tag{36}$$
$$B_2 = -\frac{2}{3}(19B_2^0 + 22B_3^0) \tag{37}$$
$$B_3 = \frac{4}{9}B_3^0 \tag{38}$$
$$C_1 = C_1^0 + \frac{2857}{2}C_2^0 + 1122C_3^0 + 1331C_4^0 \tag{39}$$
$$C_2 = -\frac{1}{18}(5033C_2^0 - 3732C_3^0 - 4356C_4^0) \tag{40}$$
$$C_3 = \frac{1}{54}(325C_2^0 + 456C_3^0 + 792C_4^0) \tag{41}$$
$$C_4 = -\frac{8}{27}C_4^0 \tag{42}$$

which are obtained with the help of Eqs.(10,33) and the four-loop $\{\beta_i\}$-terms under the $\overline{MS}$ scheme [9].

B. An application of PMC/BLM scale setting up to NNLO

We present an application of PMC/BLM scale setting up to NNLO by dealing with the total hadronic cross section in e^+e^- annihilation $R_{e^+e^-}(Q) = R(e^+e^- \to \text{hadrons})$. Explicit expression for $R_{e^+e^-}(Q)$ up to order α_s^4 under the $\overline{MS}$-scheme can be found in Ref.[22]. One finds

$$R_{e^+e^-}(Q) = 3\sum_q e_q^2\Bigg[1 + \left(a^{\overline{MS}}(Q)\right) + (1.9857 - 0.1152n_f)\left(a^{\overline{MS}}(Q)\right)^2 + \left(-6.63694 - 1.20013n_f - 0.00518n_f^2 - 1.240\frac{(\sum_q e_q)^2}{3\sum_q e_q^2}\right)\left(a^{\overline{MS}}(Q)\right)^3 + \left(-156.61 + 18.77n_f - 0.7974n_f^2 + 0.0215n_f^3 + C\frac{(\sum_q e_q)^2}{3\sum_q e_q^2}\right)\left(a^{\overline{MS}}(Q)\right)^4\Bigg], \tag{43}$$

where the coefficient C in α_s^4 is yet to be determined. At the present α_s-order, those n_f-terms that come from the light-by-light quark loops and are irrelevant to the ultra-violet cutoff do not emerge, so all n_f-terms in the above equation should be fully absorbed into α_s. After BLM scale setting up to NNLO, we obtain

$$R_{e^+e^-}(Q) = 3\sum_q e_q^2\Bigg[1 + \left(a_s^{\overline{MS}}(Q^*)\right) + \widetilde{A}\left(a_s^{\overline{MS}}(Q^{**})\right)^2 + \widetilde{\widetilde{B}}\left(a_s^{\overline{MS}}(Q^{***})\right)^3 + \widetilde{\widetilde{\widetilde{C}}}\left(a_s^{\overline{MS}}(Q^{***})\right)^4\Bigg], \tag{44}$$

where all the coefficients and effective scales can be calculated with the help of the formulae listed in the last sections. As for the unknown parameter C, its value is small [13, 23–25] and its contribution will be further suppressed by the factor $\left(\sum_q e_q)^2\right) / \left(3\sum_q e_q^2\right)$, so we directly set its value to zero at the present.

From the experimental value, $r_{e^+e^-}(31.6GeV) = \frac{3}{11}R_{e^+e^-}(31.6GeV) = 1.0527 \pm 0.0050$ [26], we obtain

$$\Lambda^{'tH}_{\overline{MS}} = 412^{+206}_{-161}\text{MeV} \tag{45}$$
$$\Lambda_{\overline{MS}} = 359^{+181}_{-140}\text{MeV} \tag{46}$$

With the help of the four loop formula (7), we obtain $\alpha_s^{\overline{MS}}(M_Z) = 0.129^{+0.009}_{-0.010}$. This value is somewhat larger than the present world average $\alpha_s^{\overline{MS}}(M_Z) = 0.1184 \pm 0.0007$ [27], however it is consistent with those obtained from e^+e^- colliders, i.e. $\alpha_s^{\overline{MS}}(M_Z) = 0.13 \pm 0.005 \pm 0.03$ by the CLEO Collaboration [28] and $\alpha_s^{\overline{MS}}(M_Z) = 0.1224 \pm 0.0039$ from the jet shape analysis [29]. One may observe that a smaller central value of the world average for $\alpha_s^{\overline{MS}}(M_Z)$ results from the measurements of τ-decays, Υ-decays, the jet production in the deep-inelastic-scattering processes, and from heavy quarkonia based on unquenched QCD lattice calculations [30]. A larger $\Lambda_{\overline{MS}}$ leads to a larger $\alpha_s^{\overline{MS}}(M_Z)$, and vice versa. If we set $\alpha_s^{\overline{MS}}(M_Z)$ to the present world average, we obtain $\Lambda^{'tH}_{\overline{MS}}|_{n_f=5} = 245^{+9}_{-10}$ MeV and $\Lambda_{\overline{MS}}|_{n_f=5} = 213^{+19}_{-8}$ MeV [6].

As a final remark, one can estimate the error caused by C with the help of the scheme-dependent equation (4). Such an analysis has been done in Ref.[8] [7]. It is

[6] Ref.[30] obtained a slightly different value of $\Lambda_{\overline{MS}}|_{n_f=5} = 215 \pm 9MeV$, which is however obtained by taking a wrong sign of $(\beta_3/2\beta_0)$ in the four-loop terms, i.e. it should be negative other than positive.

[7] Note there is a typo in Eq.(48) of Ref.[8], which should be changed to, $a_0 = a_+/\left(1 + \frac{3}{2}c_3^R a_+^3\right)^{1/3}$.

found that even if we set its value that leads to the C-term has a comparable magnitude with those without C at the fourth order, we shall only achieve an additional 2% scheme error in addition to the above experimental errors.

IV. SUMMARY

The extended renormalization group equations provide a convenient way for estimating the scale- and scheme-dependence of the QCD predictions for a physical process. The scheme dependence of a process can be reliably estimated by the scheme-equations for the extended renormalization group. In the present paper, we have presented a general solution to the scale equation of the extended renormalization group equations at the four-loop level. This formalism provides a platform for a reliable error analysis and also provides a precise definition for the asymptotic scale under any renormalization R-scheme, $\Lambda_R^{'tH}$, which is defined as the pole in the associated 't Hooft scheme.

In this paper we have given a systematic and renormalization scheme-independent method for setting PMC/BLM scales up to NNLO. The PMC provides the principle underlying BLM scale setting; they are equivalent to each other through the PMC and BLM correspondence principle. The scales can be set unambiguously by PMC/BLM, which allows us to set the renormalization scale at any required orders in obtaining a scheme-independent result. Such a scheme-independence can be adopted to derive commensurate scale relations among different observables and to find the displacements among the effective PMC/BLM scales that are derived under different schemes or conventions. The elimination of the renormalization scale ambiguity and the scheme dependence using PMC/BLM will not only increase the precision of QCD tests, but it will also increase the sensitivity of collider experiments to new physics beyond the Standard Model.

Acknowledgements: The authors would like to thank Leonardo Di Giustino for helpful discussions. This work was supported in part by the Program for New Century Excellent Talents in University under Grant No.NCET-10-0882, Natural Science Foundation of China under Grant NO.10805082 and No.11075225, and the Department of Energy contract DE-AC02-76SF00515.

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