Relating physical observables in QCD using the extended renormalization group method

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We discuss the Stückelberg-Peterman extended renormalization group equations in perturbative QCD, which express the invariance of physical observables under renormalization-scale and schemeparameter transformations. We introduce a universal coupling function that covers all possible choices of scale and scheme. Any perturbative series in QCD is shown to be equivalent to a particular point in this function. This function can be computed from a set of first-order differential equations involving the extended β functions. We propose the use of these evolution equations instead of a perturbative series for numerical evaluation of physical observables. This formalism is free of scale-scheme ambiguity and allows a reliable error analysis of higher-order corrections. It also provides a precise definition for $\Lambda_{\overline{MS}}$ as the pole in the associated 't Hooft scheme. A concrete application to $R (e^+e^- \rightarrow hadrons)$ is presented.

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I. INTRODUCTION

The scale-scheme ambiguity problem [1-3] remains one of the major obstacles impeding precise QCD predictions. Although all physical predictions in QCD should in principle be invariant under change of renormalization scale and scheme, in practice this invariance is only approximate due to the truncation of their perturbative series.

Consider the Nth-order expansion series of a physical observable R in terms of a coupling constant $\alpha_S(\mu)$ given in scheme S and at a scale μ :

$$R_{N} = r_{0} \alpha_{S}^{p}(\mu) + r_{1}(\mu) \alpha_{S}^{p+1}(\mu) + \dots + r_{N}(\mu) \alpha_{S}^{p+N}(\mu) .$$
(1)

The infinite series R_{∞} is renormalization scale-scheme invariant. However, at any finite order, the scale and scheme dependencies from the coupling constant $\alpha_S(\mu)$ and from the coefficient functions $r_i(\mu)$ do not exactly cancel, which leads to a remnant dependence in the finite series. Different choices of scale and scheme then lead to different theoretical predictions. The availability of next-to-next-to-leading-order results in QCD [4–7] has accentuated the need for study on the scale-scheme dependence.

There have been traditionally two positions on this subject. The first one is to consider the scale-scheme ambiguity as intrinsically unavoidable, and interpret the numerical fluctuations coming from different scale and scheme choices as the error in the theoretical prediction. This point of view, aside from being overly pessimistic, is also very unsatisfactory. First of all, in general we do not know how wide a range the scale and scheme parameters should vary in order to give a correct error estimate. Second, in addition to the error due to scale-scheme uncertainties there is also the error from the omitted higher-order terms. In such an approach, it is not clear whether these errors are independent or correlated. The error analysis in this context can become quite arbitrary and unreliable.

A second approach is to optimize the choice of scale and scheme according to some sensible criteria. Commonly used scale setting strategies include the principle of minimum sensitivity [1] (which also optimizes the choice of scheme), the fastest apparent convergence (FAC) criterion [2] and the Brodsky-Lepage-Mackenzie (BLM) method [3].

In this paper we use the extended renormalization group method to study the scale-scheme ambiguity problem. In this approach, a perturbative series only serves as an intermediate device for the identification of scale and scheme parameters. The ultimate prediction is obtained through evolution equations in the scale- and schemeparameter space. This approach sets the ground for a reliable error analysis and also provides a precise definition for $\Lambda_{\overline{MS}}$, where MS denotes the modified minimal subtraction scheme. Renormalization scheme invariant methods have been previously studied by Grunberg, Dhar, and Gupta [2,8], and our approach is essentially a reformulation of these methods in the language of a universal coupling function by using the Stückleberg-Peterman equations. We believe this alternative language makes the discussion of many issues on the scale-scheme ambiguity problem more transparent.

II. POWER SERIES VERSUS RENORMALIZATION GROUP

Throughout this paper we will consider the case of QCD with N_f massless quarks. We will limit ourselves to perturbative quantities that allow series expansion in the

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strong coupling constant. Nonperturbative effects such as those from instantons and possible extra complication involving structure functions or fragmentation functions are beyond the scope of this paper. Given this premise, a physical observable R in QCD can be expanded in a power series like

$$R = r_0 \alpha_0^N + r_1 \alpha_0^{N+1} + r_2 \alpha_0^{N+2} + \cdots , \qquad (2)$$

where α_0 is the bare coupling constant. In general, R can depend on several momentum scales: $R = R(\{k_i\})$. We will consider the $\{k_i\}$ to be fixed for the moment. In the above equation, r_0 is the tree-level coefficient and N is the tree-level exponent. It is well known that for a renormalizable theory such as QCD, all higher-order coefficients $\{r_i\}_{i\geq 1}$ are divergent and ill defined; hence, the power series in bare coupling constant should be considered purely formal. In other words, QCD alone does not give a direct prediction for R.

Consider now another physical quantity:

$$S = s_0 \alpha_0^M + s_1 \alpha_0^{M+1} + s_2 \alpha_0^{m+2} + \cdots$$
 (3)

As in the case of R, QCD does not provide a direct prediction for S since the coefficients $\{s_i\}_{i\geq 1}$ are also divergent However, QCD does allow us to relate S to R. The procedure is simple. We first invert Eq. (2) to obtain α_0 in terms of R:

$$\alpha_0 = \left(\frac{R}{r_0}\right)^{1/N} - \frac{r_1}{Nr_0} \left(\frac{R}{r_0}\right)^{2/N} + \cdots ; \qquad (4)$$

then we substitute this last equation into Eq. (3) to obtain

$$S = s_0 \left[\frac{R}{r_0} \right]^{M/N} + \left[s_1 - \frac{Ms_0}{Nr_0} r_1 \right] \left[\frac{R}{r_0} \right]^{(M+1)/N} + \cdots$$
(5)

For a renormalizable theory such as QCD, the expansion coefficients in this new series are expected to be finite and well defined. That is, the infinities in the divergent coefficients such as r_1 and s_1 will conspire to cancel each other, yielding a finite result.

Given a third physical quantity

$$T = t_0 \alpha_0^P + t_1 \alpha_0^{P+1} + t_2 \alpha_0^{P+2} + \cdots , \qquad (6)$$

we can similarly expand it in terms of R or S, or vice versa. We do not have a direct prediction for R, S, or T. However, if one of them is measured, QCD allows us to predict the other two.

Notice that in Eq. (5), the quantity $(R/r_0)^{1/N}$ appears repeatedly. It is convenient to give a symbol to this quantity:

$$\alpha_R \equiv \left[\frac{R}{r_0}\right]^{1/N}.$$
(7)

This quantity is known as the effective charge [2] or the effective coupling in the scheme R at the scales $\{k_i\}$. If R is a single-scale process, then α_R will depend on only one scale, but in general R and α_R can depend on more than one scale.

Similarly we can define the effective charges of S and T (or effective coupling in the schemes S and T) as

$$\alpha_{S} \equiv \left[\frac{S}{s_{0}}\right]^{1/M},$$

$$\alpha_{T} \equiv \left[\frac{T}{t_{0}}\right]^{1/P}.$$
(8)

Since the tree-level coefficients (r_0, s_0, t_0) and exponents (M, N, P) are finite and well defined, the effective charges α_R , α_S , and α_T are therefore also well defined.

In terms of effective charges, what QCD allows us to do is to relate one effective charge to another. (By putting back the tree-level coefficients and exponents, we can relate one physical observable to another.) For instance, Eq. (5) in terms of effective charges will have the form

$$\alpha_S = \alpha_R + f \alpha_R^2 + g \alpha_R^3 + \cdots, \qquad (9)$$

where the expansion coefficients f,g,... are expected to be finite.

More conventional coupling constants such as $\alpha_{\overline{\text{MS}}}(\mu)$ can also be regarded as effective charges. In fact, in dimensional regularization we have

$$\alpha_{\overline{\rm MS}}(\mu) = \alpha_0 - \left[\frac{\beta_0}{4\pi\hat{\epsilon}} + \frac{\beta_0}{4\pi} \ln\mu^2 \right] \alpha_0^2 + \cdots \qquad (10)$$

(where $1/\hat{\epsilon}=1/\epsilon+\gamma_E-\ln 4\pi$, $\epsilon=(D-4)/2$, $\beta_0=11$ $-2N_f/3$. The bare coupling constant α_0 is dimensionful in dimensional regularization. In this formula, α_0 and μ have been expressed in a preestablished mass unit.) We can regard this last equation as describing an "observable" with unit tree-level coefficient and exponent. We can expand $\alpha_{\overline{MS}}$ in terms of α_R , α_S , or α_T , or vice versa. In this context, there is no distinction between effective charges coming from physical observables or effective charges coming from more conventional coupling constants. Stretching this language, one can in fact refer to $\alpha_{\overline{MS}}$ as the effective charge of the "MS process."

Our discussion so far is valid to all orders. Realistically, we can only compute a finite number of terms in an expansion series. The direct evaluation by using a truncated series may not be the best strategy under these circumstances. Suppose we have a physical process R with $\alpha_R(Q)=0.2$ at Q=3 GeV, and we wish to evaluate the effective charge $\alpha_S(P)$ of another single-scale process S(P) at some large scale, say, $P=10^5$ GeV. The truncated series

$$\alpha_{S}(P) = \alpha_{R}(Q) + f(P,Q)\alpha_{R}^{2}(Q)$$
(11)

will have a large value of f(P,Q) and higher-order contributions cannot be neglected. In fact, it is known that for a large enough value of P, this truncated series will give a negative value for $\alpha_s(P)$.

What if S = R in the above discussion? That is, what if we want to evaluate $\alpha_R (10^5 \text{ GeV})$ from $\alpha_R (3 \text{ GeV})$? The answer is clear: we should use the renormalization group equation to evolve $\alpha_R(Q)$ from Q = 3 GeV to $Q = 10^5$ GeV. Given the β function

$$\beta_R(\alpha_R) = \frac{d}{d \ln Q^2} \left(\frac{\alpha_R}{4\pi} \right) = -\beta_0 \left(\frac{\alpha_R}{4\pi} \right)^2 + \cdots , \qquad (12)$$

we can use it for the evolution of α_R . To first order we obtain

$$\alpha_{R}(P) = \frac{\alpha_{R}(Q)}{1 + (\beta_{0}/4\pi)\alpha_{R}(Q)\ln(P^{2}/Q^{2})} .$$
(13)

This result is much more reliable than the one given by the truncated series. In fact, $\alpha_R(P)$ now remains positive for arbitrarily large values of P.

Why is the renormalization group method better than the direct evaluation of the truncated series? The answer is that along the evolution trajectory the scale is changed in a continuous fashion, thus avoiding the presence of dissimilar scales and large coefficients.

Let us come back to the case of two different processes. Given two effective charges $\alpha_R(Q)$ and $\alpha_S(P)$, each one of them can be characterized by its respective β function:

$$\beta_{R}(\alpha_{R}) = \frac{d}{d \ln Q^{2}} \left[\frac{\alpha_{R}}{4\pi} \right]$$

$$= -\beta_{0} \left[\frac{\alpha_{R}}{4\pi} \right]^{2} -\beta_{1} \left[\frac{\alpha_{R}}{4\pi} \right]^{3} -\beta_{2}^{R} \left[\frac{\alpha_{R}}{4\pi} \right]^{4} + \cdots,$$
(14)
$$\beta_{S}(\alpha_{S}) = \frac{d}{d \ln P^{2}} \left[\frac{\alpha_{S}}{4\pi} \right]$$

$$= -\beta_{0} \left[\frac{\alpha_{S}}{4\pi} \right]^{2} -\beta_{1} \left[\frac{\alpha_{S}}{4\pi} \right]^{3} -\beta_{2}^{S} \left[\frac{\alpha_{S}}{4\pi} \right]^{4} + \cdots.$$

The universality of the first two β -function coefficients β_0 and β_1 is a well-known fact. Stevenson [1] has shown that a scheme can be parametrized by its higher-order β coefficients. Therefore, the *R* scheme is characterized by $\{\beta_n^R\}_{n\geq 2}$, and the *S* scheme by $\{\beta_n^S\}_{n\geq 2}$. In the expansion series of $\alpha_S(P)$ in terms of $\alpha_R(Q)$

$$\alpha_{S}(P) = \alpha_{R}(Q) + f(P,Q)\alpha_{R}^{2}(Q) + g(P,Q)\alpha_{R}^{3}(Q) + \cdots ,$$
(15)

we know that we need a scale $Q \sim P$ to have a reasonable expansion coefficient f(P,Q). However, this may not be enough to guarantee a good convergence if S and R are very different schemes. That is, if the β function coefficients β_2^R and β_2^S are very different, then the expansion coefficients such as g(P,Q) can still be large, rendering the truncated series useless. (The detailed dependence of the expansion coefficient on the scale and scheme parameters will be obtained later.)

The strategy to follow is now clear. We should evolve $\alpha_R(Q)$ "adiabatically" into $\alpha_S(P)$, not only in scale but also in scheme. Along the evolution trajectory, no dissimilar scales or schemes are involved; thus, we can expect the result to be more reliable. We need new equations and β functions that allow us to evolve the scheme parameters $\{\beta_n^R\}$ into $\{\beta_n^S\}$. This will be the subject of the next section.

Let us conclude this section with a comment on error

estimation. Conventionally one can estimate the error of a finite series by estimating the next-order coefficient. However, when the power series is unreliable due to largely mismatched scales and schemes, so the corresponding error estimate will be. We will see that in the extended renormalization group method we can first estimate the next-order scheme parameter, and then translate the scheme uncertainty into the error estimate for a physical observable.

III. THE UNIVERSAL COUPLING FUNCTION IN QCD

In this section we will set up the appropriate notation and define the universal coupling function. Given an effective charge $\alpha_R = \alpha_R(\{k_i\})$, we define its fundamental β function (or scale β function) to be

$$\beta_{R}(\alpha_{R}) = \frac{d}{d \ln \lambda^{2}} \left[\frac{\alpha_{R}(\{\lambda k_{i}\})}{4\pi} \right]$$
$$= -\beta_{0} \left[\frac{\alpha_{R}}{4\pi} \right]^{2} - \beta_{1} \left[\frac{\alpha_{R}}{4\pi} \right]^{3} - \beta_{2}^{R} \left[\frac{\alpha_{R}}{4\pi} \right]^{4} + \cdots$$
(16)

The first two coefficients β_0 and β_1 are universal, whereas all higher-order coefficients $\{\beta_n^R\}_{n\geq 2}$ are process dependent. It will be very convenient to use the first two coefficients of the beta functions to rescale the coupling constant and the scale parameter $\ln \lambda^2$. [The quantity λ effectively parametrizes the overall scale of a process. For single-scale processes, the derivative with respect to the scale parameter can be replaced by the derivative with respect to the scale of the process, as given in Eq. (14).]

Let us define the rescaled coupling constant and the rescaled scale parameter as

$$a_R = \frac{\beta_1}{\beta_0} \frac{\alpha_R}{4\pi} , \ \tau = \frac{\beta_0^2}{\beta_1} \ln \lambda^2 .$$
 (17)

The rescaled β function takes the canonical form

$$\beta_R(a_R) = \frac{da_R}{d\tau} = -a_R^2 (1 + a_R + c_2^R a_R^2 + c_3^R a_R^3 + \cdots) ,$$
(18)

with $c_n^R = \beta_n^R \beta_0^{n-1} / \beta_1^n$ for n = 2, 3, ... This rescaling process serves to "unitarize" the expansion coefficients. (Our definition of the scheme parameters differs slightly from Stevenson's [1].) For a well-behaved scheme in QCD, we would expect its β -function expansion to roughly resemble a geometrical series, at least for the first few coefficients. In fact, for the MS scheme we have $c_2^{MS} = \beta_2^{MS} \beta_0 / \beta_1^2$, where [9]

$$\beta_0 = 11 - \frac{2}{3}N_f ,$$

$$\beta_1 = 102 - \frac{38}{3}N_f ,$$

$$\beta_2^{\overline{\text{MS}}} = \frac{2857}{2} - \frac{5033}{18}N_f + \frac{325}{54}N_f^2 ,$$
(19)

The universal coupling function $a(\tau, \{c_i\})$ is the extension of an ordinary coupling constant to include the dependence on scheme parameters. It is required to satisfy the scale evolution equation

$$\beta(a, \{c_i\}) = \frac{\delta a}{\delta \tau} = -a^2(1 + a + c_2 a^2 + c_3 a^3 + \cdots)$$
 (20)

for all values of $\{c_i\}$.

The scheme β functions are defined as

$$\beta_{(n)}(a, \{c_i\}) \equiv \frac{\delta a}{\delta c_n} .$$
⁽²¹⁾

As shown by Stevenson [1], these extended β functions can be defined in terms of the fundamental β function. Indeed, the commutativity of second partial derivatives

$$\frac{\delta^2 a}{\delta \tau \delta c_n} = \frac{\delta^2 a}{\delta c_n \delta \tau}$$
(22)

implies

$$\frac{\delta\beta_{(n)}}{\delta\tau} = \frac{\delta\beta}{\delta c_n} , \qquad (23)$$

$$\beta \beta'_{(n)} = \beta_{(n)} \beta' - a^{n+2} , \qquad (24)$$

where $\beta'_{(n)} = \partial \beta_{(n)} / \partial a$ and $\beta' = \partial \beta / \partial a$. From here

$$\beta^2 \left[\frac{\beta_{(n)}}{\beta} \right] = -a^{n+2} ; \qquad (25)$$

therefore

$$\beta_{(n)}(a, \{c_i\}) = \frac{\delta a}{\delta c_n} = -\beta(a, \{c_i\}) \int_0^a dx \frac{x^{n+2}}{\beta^2(x, \{c_i\})} ,$$
(26)

where the lower limit of the integral has been set to satisfy the boundary condition

$$\beta_{(n)} = O(a^{n+1})$$
 (27)

That is, a change in the scheme parameter c_n can only affect terms of order a^{n+1} and higher in the evolution of the universal coupling function [1].

We define the universal coupling function $a(\tau, \{c_i\})$ as the solution to the evolution equations (20) and (26) with the boundary condition

$$a(0, \{0\}) = \infty . (28)$$

Notice that the evolution equations contain no explicit reference to QCD parameters such as the number of colors or the number of flavors. Therefore, aside from its infinite dimensional character, $a(\tau, \{c_i\})$ is just a mathematical function such as, say, Bessel functions or any other special function. Truncation of the fundamental β function simply corresponds to evaluating $a(\tau, \{c_i\})$ is a subspace where higher-order c_i are zero (Fig. 1).



FIG. 1. Pictorial representation of the universal coupling function $a(\tau, \{c_i\})$, where τ is the scale parameter and $\{c_i\}$ the scheme parameters.

In the next section we will explain how to use the universal coupling constant and the scale and scheme β functions to relate various effective charges. To conclude this section, let us point out that any physical quantity R can be expressed as a power series in terms of the universal coupling constant. The invariance of R with respect to change of scale and scheme parameters is described by the equations

$$\frac{\delta R}{\delta \tau} = 0 , \qquad (29)$$
$$\frac{\delta R}{\delta c_n} = 0 .$$

These equations have first been studied by Stückelberg and Peterman [10].

IV. RELATING TWO EFFECTIVE CHARGES

Any given effective charge a_R can be expressed in terms of the universal coupling function. Since $a_R(\{k_i\})$ and $a(\tau, \{c_i^R\})$ satisfy the same scale evolution equation [compare Eq. (18) to Eq. (20)], there exists a value of $\tau = \tau_R$ for which

$$a_{R} = a(\tau_{R}, \{c_{i}^{R}\}) .$$
(30)

We will call τ_R the scale parameter of R. Notice that, although the scheme parameters $\{c_i^R\}$ can be obtained from QCD by computing the coefficients in the fundamental β function, the value of the scale parameter τ_R is not provided by the theory. This is expected since we know QCD alone does not give a prediction for a_R . A measurement of a_R will allow us to obtain τ_R .

Once a_R (and therefore τ_R) is measured, QCD allows us to predict the value of other effective charges. In order to evolve the universal coupling function from a_R to, say, a_S , we need to know the scale and scheme parameters ($\tau_S, \{c_s^S\}$) of a_S . As we know, the expansion series

$$a_{\rm S} = a_{\rm R} + f_2 a_{\rm R}^2 + f_3 a_{\rm R}^3 + \cdots$$
(31)

is unreliable for evaluating a_S directly. However, this series will allow us to obtain the scale and scheme parameters of a_S from those of a_R .

To make this contact transparent, let us expand the universal coupling function in Taylor series around the point $(\tau_R, \{c_i^R\})$:

$$a_{S} = a (\tau_{S}, \{c_{i}^{S}\}) = a (\tau_{R} + \overline{\tau}, \{c_{i}^{R} + \overline{c}_{i}\})$$

$$= a_{R} + \left[\frac{\delta a}{\delta \tau}\right]_{R} \overline{\tau} + \left[\frac{\delta a}{\delta c_{n}}\right]_{R} \overline{c}_{n}$$

$$+ \frac{1}{2!} \left[\left[\frac{\delta^{2} a}{\delta \tau^{2}}\right]_{R} \overline{\tau}^{2} + 2 \left[\frac{\delta^{2} a}{\delta \tau \delta c_{n}}\right]_{R} \overline{\tau} \overline{c}_{n}$$

$$+ \left[\frac{\delta^{2} a}{\delta c_{n} \delta c_{m}}\right]_{R} \overline{c}_{n} \overline{c}_{m} \right]$$

$$+ \frac{1}{3!} \left[\left[\frac{\delta^{3} a}{\delta \tau^{3}}\right]_{R} \overline{\tau}^{3} + \cdots \right] + \cdots, \quad (32)$$

where

$$\overline{\tau} = \tau_S - \tau_R , \qquad (33)$$
$$\overline{c}_n = c_n^S - c_n^R ,$$

and the subscript R next to the partial derivatives means they are evaluated at the point $(\tau_R, \{c_i^R\})$. To order a^4 , we only need the partial derivatives

$$\left[\frac{\delta a}{\delta \tau}\right] = \beta = -a^2 - a^3 - c_2 a^4 + O(a^5) ,$$

$$\left[\frac{\delta a}{\delta c_2}\right] = \beta_{(2)} = a^3 + O(a^5) ,$$

$$\left[\frac{\delta a}{\delta c_3}\right] = \beta_{(3)} = \frac{1}{2}a^4 + O(a^5) ,$$

$$\left[\frac{\delta^2 a}{\delta \tau^2}\right] = 2a^3 + 5a^4 + O(a^5) ,$$

$$\left[\frac{\delta^2 a}{\delta \tau^{\delta c_2}}\right] = -3a^4 + O(a^5) ,$$

$$\left[\frac{\delta^3 a}{\delta \tau^3}\right] = -6a^4 + O(a^5) .$$
(34)

After grouping all the terms in powers of $a = a_R$, we obtain

$$a_{S} = a_{R} - \bar{\tau}a_{R}^{2} + (\bar{c}_{2} - \bar{\tau} + \bar{\tau}^{2})a_{R}^{3} + (\frac{1}{2}\bar{c}_{3} - (c_{2}^{R} + 3\bar{c}_{2})\bar{\tau} + \frac{5}{2}\bar{\tau}^{2} - \bar{\tau}^{3})a_{R}^{4} + O(a_{R}^{5}) , \qquad (35)$$

where $\overline{\tau}$ and \overline{c}_n are as given in Eq. (33). The coefficients of this formula have been previously obtained by Maxwell and Stevenson in a slightly different notation [11,12]. Notice the occurrence of $\overline{\tau}$ and \overline{c}_i in all higher-order coefficients. By using the evolution equations, we are effectively performing a partial resummation of the perturbative series to all orders. By matching this last equation with Eq. (31), we can identify the scale and scheme parameters of a_S order by order. For instance,

$$\tau_{S} = \tau_{R} - f_{2} ,$$

$$c_{2}^{S} = c_{2}^{R} - f_{2} - f_{2}^{2} + f_{3} ,$$

$$c_{3}^{S} = c_{3}^{R} - 2f_{2}c_{2}^{R} + f_{2}^{2} + 4f_{2}^{3} - 6f_{2}f_{3} + 2f_{4} .$$
(36)

Let us summarize here the necessary steps to evolve a_R to a_S .

(1) Obtain the scheme parameters of a_R by calculating the coefficients of its fundamental β equation. [In the case of $\overline{\text{MS}}$ scheme these parameters are known. See Eq. (19).]

(2) By Feynman diagram calculation, obtain the expansion series of a_S in terms of a_R . [See Eq. (31).]

(3) Identify the scale and scheme parameters of a_s in terms of those of a_R . [See Eq. (36).]

(4) Evolve a_R to a_S by using the Stückelberg-Peterman evolution equations (20) and (26). The final result will not depend on the choice of the evolution path.

A concrete application of this procedure to $R(e^+e^- \rightarrow hadrons)$ will be presented later. But first, let us explain the meaning of the 't Hooft scheme and the 't Hooft scale.

V. THE 't HOOFT SCHEME AND SCALE

The universal coupling function adopts a particularly simple form when all the scheme parameters are zero. In fact, the 't Hooft scheme [13] coupling constant $a_{\text{'tH}}(\tau) \equiv a(\tau, \{0\})$ is exactly given by the solution of

$$\frac{1}{a_{tH}} + \log\left[\frac{a_{tH}}{1 + a_{tH}}\right] = \tau .$$
(37)

(The optimization of QCD perturbative series in this scheme has been studied by Maxwell [11].) Notice that because of the boundary condition $a(0,\{0\})=\infty$, the 't Hooft coupling constant presents a singularity at $\tau=0$.

For any single-scale effective charge $a_R(\mu)$ there exists a scale $\mu = \Lambda_R^{'tH}$ for which the scale parameter $\tau_R = 2\beta_0^2\beta_1^{-1}\log(\mu/\Lambda_R^{'tH})$ vanishes. We will call $\Lambda_R^{'tH}$ the 't Hooft scale¹ of the *R* scheme. To understand the meaning of the 't Hooft scale, let us consider the $\overline{\text{MS}}$ scheme coupling constant as an example:

$$a_{\overline{\mathrm{MS}}}(\mu) = a \left[\frac{2\beta_0^2}{\beta_1} \log(\mu / \Lambda_{\overline{\mathrm{MS}}}^{\underline{\mathrm{'IH}}}), \{c_i^{\overline{\mathrm{MS}}}\} \right].$$
(38)

Notice that a priori we do not know the behavior of $a_{\overline{\text{MS}}}(\mu)$ at $\mu = \Lambda_{\overline{\text{MS}}}^{\underline{\text{'H}}}$: it could be infinite, finite or simply not well defined. However, $\mu = \Lambda_{\overline{\text{MS}}}^{\underline{\text{'H}}}$ is the pole in the 't Hooft scheme associated² with the MS scheme:

¹For multiple-scale processes, the submanifold where the scale parameter vanishes defines the "'t Hooft surface."

²There are an infinite number of 't Hooft schemes, differing only by the value of the 't Hooft scale $\Lambda'^{\text{'H}}$. The word "associated" here means we are choosing the particular 't Hooft scheme that shares the same 't Hooft scale with the $\overline{\text{MS}}$ scheme: $\Lambda'^{\text{'H}} = \Lambda'^{\text{'H}}_{\overline{\text{MS}}}$.





FIG. 2. Graphical representation of the various errors involved. For the measurement of Λ_{MS}^{tH} (or equivalently Λ_{R}^{tH}) the input experimental error must be combined with the scheme uncertainty. For the prediction of $a_R(\tau)$, the error in Λ_{MS}^{tH} must be combined with the scheme uncertainty.

$$a_{\text{tH}-\overline{\text{MS}}}(\mu) \equiv a \left[\frac{2\beta_0^2}{\beta_1} \log(\mu/\Lambda_{\overline{\text{MS}}}^{\text{tH}}), \{0\} \right], \quad (39)$$

because $a(0, \{0\}) = \infty$ by boundary condition. Since the 't Hooft scheme is completely free of higher-order corrections, this provides a precise definition for $\Lambda_{\overline{MS}}$.

As stated before, an experimental measurement of a_R leads us to the measurement of τ_R , which in turn gives a value for $\Lambda_R^{'tH}$. In Fig. 2 we show the various experimental and theoretical errors involved in the analysis. For the measurement of $\Lambda_R^{'tH}$, the input experimental error must be combined with the scheme uncertainty to give the error estimate for $\Lambda_R^{'tH}$. Similarly, for the prediction of $\alpha_R(\tau)$ the error from $\Lambda_R^{'tH}$ must be combined with the scheme uncertainty in order to give the prediction error.

VI. APPLICATION TO R ($e^+e^- \rightarrow$ HADRONS)

In this section we present a concrete application to the total hadronic cross section in e^+e^- annihilation $R(Q) = R(e^+e^- \rightarrow \text{hadrons})$ recently calculated to order α^3 [4,6]. (See also the recent analysis in Refs. [4], [14], and [15].) From Refs. [4,6], for five light-quark flavors we have

$$R(Q) = \frac{11}{3} \left[1 + \frac{\alpha_{\overline{\text{MS}}}(Q)}{\pi} + 1.4092 \left[\frac{\alpha_{\overline{\text{MS}}}(Q)}{\pi} \right]^2 - 12.8046 \left[\frac{\alpha_{\overline{\text{MS}}}(Q)}{\pi} \right]^3 \right]$$
$$\equiv \frac{11}{3} \left[1 + \frac{\alpha_R(Q)}{\pi} \right]. \tag{40}$$

Let us perform some preliminary analysis. By rescaling the effective charges appropriately [see Eq. (17)], we obtain the relation

$$a_R(Q) = a_{\overline{\text{MS}}}(Q) + 1.1176a_{\overline{\text{MS}}}^2(Q) - 8.05426a_{\overline{\text{MS}}}^3(Q)$$
 .
(41)

Notice that in the right-hand side the scale argument of $a_{\overline{\text{MS}}}(\mu)$ has been set to be $\mu = Q$. In general, this needs not to be the case. When μ is left to be free, the relation between $a_R(Q)$ and $a_{\overline{\text{MS}}}(\mu)$ is given by

$$a_{R}(Q) = a_{\overline{\text{MS}}}(\mu) + [1.1176 - 3.0402 \ln(Q/\mu)] a_{\overline{\text{MS}}}^{2}(\mu) + [-8.05426 - 9.8358 \ln(Q/\mu) + 9.2430 \ln^{2}(Q/\mu)] a_{\overline{\text{MS}}}^{3}(\mu) .$$
(42)

Applying the formulas in Eq. (36) and knowing that $\tau_R = 2\beta_0^2\beta_1^{-1}\ln(Q/\Lambda_R^{'tH})$ and $\tau_{\overline{MS}} = 2\beta_0^2\beta_1^{-1}\ln(\mu/\Lambda_{\overline{MS}}^{'tH})$, we arrive at the relations

$$\Lambda_R^{'tH} = 1.4443 \Lambda_{MS}^{'tH}, \ c_2^R = -9.4932.$$
 (43)

Notice that, as one would expect, these results are independent of the scales Q and μ that we started with. In fact, we could use any scale and scheme in the right-hand side of Eq. (42), and always arrive to the same values of scale parameters for a_R and a consistent ratio of the 't Hooft scales.

Experimentally [16] we have

$$r(31.6 \text{ GeV}) = \frac{3}{11}R(31.6 \text{ GeV}) = 1.0527 \pm 0.0050$$
, (44)

which gives

$$a_R(31.6 \text{ GeV}) = 0.0665 \pm 0.0063$$
 (45)

We will now use this information to obtain values for $\Lambda_{MS}^{'tH}$. We have to take into account the scheme uncertainty in addition to the experimental error in order to quote a correct error estimate for $\Lambda_{MS}^{'tH}$ (see Fig. 3). The scheme uncertainty of R can be quantified by a reasonable esti-



FIG. 3. Measurement of $\Lambda_{MS}^{'H}$ from the experimental result of $a_R(31.6 \text{ GeV})$. We have parametrized the scheme uncertainty with a value $c_3^R = 100$. The scheme, experimental and total errors are, respectively, given by $\Delta_{sch} = (\tau_5 - \tau_3)/2$, $\Delta_{exp} = (\tau_6 - \tau_2)/2$ and $\Delta_{tot} = (\tau_7 - \tau_1)/2$. There is a one-to-one relationship between τ and $\Lambda_{MS}^{'H}$ given by $\tau = 2\beta_0^2\beta_1^{-1} \log(31.6 \text{ GeV}/1.4443\Lambda_{MS}^{'H})$.

mate of its next scheme parameter: c_3^R . West [17] has put an estimate $r_4 = -158.6$ for the coefficient of $(\alpha_{\overline{\text{MS}}}(Q)/\pi)^4$ in Eq. (40). After rescaling, this leads to a value $\overline{c}_3 = c_3^R - c_3^{\overline{\text{MS}}} = -99.474$. Assuming $c_3^{\overline{\text{MS}}}$ is of order unity, we conclude that $|c_3^R| \sim 100$. Although we have some reservation on West's estimate (see Ref. [18]), we shall nonetheless use it to illustrate our procedure. A better estimate of c_3^R will lead to a better error estimate for $\Lambda_{\overline{\text{MS}}}^{'\text{H}}$.

In Fig. 3 we show the universal charge for $a_0(\tau) = a(\tau, \{c_2 = c_2^R, c_3 = c_4 = \cdots = 0\})$ and its evolution under a scheme uncertainty $c_3 = \pm 100$ to $a_{\pm}(\tau) = a(\tau, \{c_2 = c_2^R, c_3 = \pm 100, c_4 = c_5 = \cdots = 0\})$.

The evolution in the scheme parameters are dictated by

$$\frac{\delta a}{\delta c_2} = \beta_{(2)} = -\beta \int_0^a dx \frac{x^4}{\beta^2} \sim a^3 + O(a^5) ,$$

$$\frac{\delta a}{\delta c_3} = \beta_{(3)} = -\beta \int_0^a dx \frac{x^5}{\beta^2} \sim \frac{1}{2}a^4 + O(a^5) .$$
 (46)

For our region of interest $(a \sim 0.07)$ the first term in each expansion series suffices. But we should use the full integro-differential equation whenever we want to evolve *a* to a higher-value region. This will not only improve the accuracy of our result, but also will respect the commutativity of the second-order partial derivatives of *a* and thus ensure the independence of the result on the choice of integration path.

To obtain the various scale parameters in Fig. 3, we can evolve their corresponding values of a_R to the 't Hooft scheme (switching off all scheme parameters) and then use Eq. (37) to get the value for the particular τ . Let us illustrate the procedure for τ_7 . If we denote

$$a_{+} = a(\tau_{7}, c_{2}^{R}, c_{3}^{R}, 0, ...) = 0.06016 ,$$

$$a_{0} = a(\tau_{7}, c_{2}^{R}, 0, 0, ...) ,$$

$$a_{\cdot_{tH}} = a(\tau_{7}, 0, 0, 0, ...) ,$$
(47)

then the solutions to the evolution equations in (46) are given by

$$a_{0} = \frac{a_{+}}{(1 + \frac{3}{2}c_{3}^{R}a_{+}^{3})^{1/2}},$$

$$a_{tH} = \frac{a_{0}}{(1 + 2c_{2}^{R}a_{0}^{2})^{1/2}}.$$
(48)

Using these equations and Eq. (37), we obtain a value of $\tau_7 = 13.379$. Other scale parameters can be calculated in a similar way. In Fig. 3 we show the various errors involved in this analysis. Numerically we find the experimental, scheme, and total errors for τ to be

$$\Delta \tau_{\text{expt}} = (\tau_6 - \tau_2)/2 = 1.41 ,$$

$$\Delta \tau_{\text{sch}} = (\tau_5 - \tau_3)/2 = 0.22 ,$$

$$\Delta \tau_{\text{tot}} = (\tau_7 - \tau_1)/2 = 1.63 .$$

(49)

These errors can be translated into uncertainties in Λ_{MS}^{tH} since there is a one-to-one correspondence between τ and

 $\Lambda_{MS}^{'tH}$. [The ratio between $\Lambda_R^{'tH}$ and $\Lambda_{MS}^{'tH}$ is given in Eq. (43).] We can see that most error comes from the experimental error and the scheme error are highly uncorrelated since $\Delta \tau_{tot} \sim \Delta \tau_{expt} + \Delta \tau_{sch}$. Numerically we obtain $\tau_1 = 10.129, \tau_4 = 11.666$, and $\tau_7 = 13.379$. Knowing that

$$\tau = \frac{2\beta_0^2}{\beta_1} \log \left[\frac{31.6 \text{ GeV}}{1.4443\Lambda_{\text{MS}}^{'\text{IH}}} \right], \tag{50}$$

we arrive at the following result for Λ_{MS}^{2H} :

$$\Lambda_{\rm MS}^{\rm tH} = 472^{+310}_{-204} \,\,{\rm MeV} \,\,. \tag{51}$$

If there were no experimental error, the estimated scheme uncertainty would lead to³ $\Lambda_{MS}^{'tH} = 472^{+35}_{-33}$ MeV.

As a second application of our formalism, we will show next how to use the experimental result of a_R (31.6 GeV) to predict other effective charges. Specifically, we will give a prediction for $a_{\overline{\text{MS}}}(M_Z)$, where $M_Z = 91.173 \text{ GeV}$ is the mass of the Z boson. The evolution of $a_R(31.6)$ GeV) to $a_{\overline{\text{MS}}}(M_Z)$ is illustrated in Fig. 4. Notice that the experimental and the scheme uncertainties confine the correct result for a_R into an approximate parallelogram ABCD. We can then evolve this parallelogram into any other scheme and scale. We will use $c_3^R = \pm 100$ and $c_3^{MS} = \pm 1$ to estimate the scheme uncertainties in a_R and $a_{\overline{\text{MS}}}$. For $a_{\overline{\text{MS}}}(M_Z)$, the parallelogram *ABCD* is evolved into the parallelogram A'B'C'D'. Notice the inversion of the orientation of the new parallelogram due to the opposite signs of c_2^R and $c_2^{\overline{MS}}$. Notice also the absence of scheme uncertainty in the 't Hooft scheme.

From $\tau_A = 10.129$ and $\tau_C = 13.379$ and knowing that $\tau_{\overline{MS}} = \tau_R - \overline{\tau}$ with $\overline{\tau} = 2\beta_0^2 \beta_1^{-1} [\log(M_Z / \Lambda_{\overline{MS}}^{\text{tH}}) - \log (31.6 \text{ GeV} / \Lambda_R^{\text{tH}})] = 4.339$, we find $\tau_{A'} = 14.468$ and $\tau_{C'} = 17.718$. To evaluate $a_{A'} = a(\tau_{A'}, c_2^{\overline{MS}} = 0.92766, c_3^{\overline{MS}} = 1, 0, \ldots)$ and $a_{C'} = a(\tau_{C'}, c_2^{\overline{MS}} = 0.92766, c_3^{\overline{MS}} = -1, 0, \ldots)$ we can use the following steps. We will show the procedure for $a_{A'}$.

(1) Generate the 't Hooft scheme coupling $a_{tH} = a(\tau_{A'}, 0, ...)$ by solving iteratively

$$a_{tH} = \frac{1}{\tau_{A'} + \log(1 + 1/a_{th})}$$
 (52)

(2) Evolve a_{tH} to $a_0 = a(\tau_{A'}, c_2^{\overline{MS}}, 0, ...)$ by displacing in c_2 :

$$a_0 = \frac{a_{^{\prime}\text{tH}}}{(1 - 2c_2^{\overline{\text{MS}}} a_{^{^{\prime}\text{tH}}}^2)^{1/2}} .$$
(53)

(3) Evolve a_0 to $a_{A'} = a(\tau_{A'}, c_2^{\overline{\text{MS}}}, c_3^{\overline{\text{MS}}} = 1, 0, ...)$ by displacing in c_3 :

³In terms of the definition of $\Lambda_{\overline{\text{MS}}}$ as given by the Particle Data Group [19] (see also Sec. VI), the corresponding values are $\Lambda_{\overline{\text{MS}}} = 411^{+270}_{-178} \text{ MeV}$ and $\Lambda_{\overline{\text{MS}}} = 411^{+270}_{-29} \text{ MeV}$.



FIG. 4. Prediction of $a_{\overline{MS}}(M_Z)$ from the experimental result of $a_R(31.6 \text{ GeV})$. By using the extended renormalization group equations, the quasi-parallelogram *ABCD* is evolved into the quasiparallelogram *A'B'C'D'*. Notice that inversion of the orientation of the parallelograms due to the opposite signs of c_3^R and $c_3^{\overline{MS}}$. Notice also the absence of scheme uncertainty in the 't Hooft scheme.

$$a_{A'} = \frac{a_0}{(1 - \frac{3}{2}c_3^{\overline{\text{MS}}}a_0^3)^{1/3}} .$$
 (54)

From here we obtain $a_{A'}=0.05772$ and $a_{C'}=0.04818$. Hence, we arrive at the prediction

$$a_{\overline{\text{MS}}}(M_Z) = 0.0530 \pm 0.0048$$
, (55)

or equivalently,⁴

$$\alpha_{\overline{\text{MS}}}(M_Z) = 0.132 \pm 0.012$$
 (56)

VII. RELATED COMMENTS

Let us show next that our formalism is closely related to the FAC criterion when only the next-to-leading-order coefficient is known. We define FAC here as the condition of a vanishing next-to-leading-order coefficient.

Given

$$a_R(Q) = a_{\overline{\mathrm{MS}}}(\mu) - \overline{\tau} a_{\overline{\mathrm{MS}}}^2(\mu) , \qquad (57)$$

with

$$\overline{\tau} = 2\beta_0^2 \beta_1^{-1} [\log(Q/\Lambda_R^{'\text{tH}}) - \log(\mu/\Lambda_{\overline{\text{MS}}}^{'\text{tH}})] , \qquad (58)$$

and assuming a complete lack of knowledge of the scheme parameters $\{c_i^{MS}\}$ and $\{c_i^R\}$, we cannot do much better than to approximate

$$a_{R}(Q) = a \left[\frac{2\beta_{0}^{2}}{\beta_{1}} \log(Q/\Lambda_{R}^{'tH}), \{0\} \right],$$

$$a_{\overline{\text{MS}}}(\mu) = a \left[\frac{2\beta_{0}^{2}}{\beta_{1}} \log(\mu/\Lambda_{\overline{\text{MS}}}^{'tH}), \{0\} \right],$$
(59)

and absorb the uncertainty from scheme parameters into our theoretical error. However, the last two equations imply that

$$a_{R}(Q) = a_{\overline{\mathrm{MS}}} \left[\mu = \frac{\Lambda_{\overline{\mathrm{MS}}}^{'\mathrm{tH}}}{\Lambda_{R}^{'\mathrm{tH}}} Q \right] \,. \tag{60}$$

Hence, by setting the coefficient $\overline{\tau}$ in Eq. (57) to zero, we obtain the correct ratio for the two scales. Actually, this holds true in general: by applying the FAC criterion, we always obtain the correct ratio of the definition $R \equiv r_0 \alpha_R^p$ has the advantage that r_0 and p are renormalization scale and scheme invariant quantities.

However, the FAC definition of effective charges α_R by $R \equiv r_0 \alpha_R^p$ is not the only possibility. Other definitions have been discussed in Ref. [21]. As we have shown in this paper any convenient choice of effective charge can be used to relate physical observables. In fact, we can apply the extended renormalization group technique to the effective BLM charge [3] defined in the following manner. Given two physical quantities R and R' computed in a particular scheme,

$$R(Q) = r_0(Q)\alpha^{p}(\mu) + [r_{10}(Q) + r_{11}(Q,\mu)\beta_0]\alpha^{p+1}(\mu) + \cdots,$$

$$R'(Q') = r'_0(Q')a^{p'}(\mu')$$
(61)

+
$$[r'_{10}(Q')+r'_{11}(Q',\mu')\beta_0]\alpha^{p'+1}(\mu')+\cdots,$$

where $\beta_0 = 11 - \frac{2}{3}N_f$ is the first β function coefficient, we can define their "effective BLM charges" by

$$R(Q) = r_0(Q)\alpha_{R-BLM}^p(Q) + r_{10}(Q)\alpha_{R-BLM}^{p+1}(Q) + \dots ,$$

$$R'(Q') = r'_0(Q')\alpha_{R'-BLM}^{p'}(Q') + r'_{10}(Q')\alpha_{R'-BLM}^{p'+1}(Q') + \dots ,$$
(62)

$$+ \dots ,$$

with $\alpha_{R-BLM}(Q) = \alpha(\mu^*)$ where μ^* is the solution of $r_{11}(Q,\mu^*)=0$, and similarly $\alpha_{R'-BLM}(Q')=\alpha(\mu'^*)$ where μ'^* is the solution of $r'_{11}(Q',\mu'^*)=0$. With this choice of scale, vacuum polarization contributions are associated with the charge rather than the expansion coefficients, and the scale tends to reflect the mass of the virtual gluons. The BLM method is particularly advantageous for setting the scale when one only has low-order calculations available since it automatically resumes the higher-order contributions associated with vacuum polarization insertions.

We can now apply the evolution equations to $\alpha_{R-BLM}(Q)$ and evolve it to $\alpha_{R'-BLM}(Q')$. The evolution in the scheme parameters maintains the BLM condition that the next-to-leading-order coefficient is flavor independent. In fact, both the FAC and BLM definitions are consistent with evolution in the scheme and scale parameters.

⁴This value is higher than the world average $\alpha_{\overline{\text{MS}}}(M_Z) = 0.1134 \pm 0.0035$ quoted by the Particle Data Group [19] but still consistent with other quoted values for $\alpha_{\overline{\text{MS}}}(M_Z)$. For instance, $\alpha_{\overline{\text{MS}}}(M_Z) = 0.118 \pm 0.008$ is obtained by OPAL [20]. The detailed analysis of consistency between the various experimental results is beyond the purpose of this paper.

By noting that the scheme β function are higher powered in a, $\beta_{(n)} \sim O(a^{n+1})$, and thus scheme effects become negligible at large τ , one can obtain a compact formula that gives the universal coupling function $a(\tau, \{c_i\})$ implicitly in terms of the scale and scheme parameters. This has been done by Grunberg [2] and Dhar and Gupta [8] in their study of renormalization scheme invariant method. In our notation the formula is given by

$$\tau = \frac{1}{a} + \ln\left(\frac{a}{1+a}\right) + \int_0^a dx \left[\frac{1}{\beta(x, \{c_i\})} + \frac{1}{x^2(1+x)}\right].$$
(63)

Finally, let us obtain the relation between $\Lambda_{\overline{MS}}^{\underline{'H}}$ and a commonly used definition of $\Lambda_{\overline{MS}}$. The expansion of $\alpha_{\overline{MS}}(\mu)$ can be obtained by inverting the above formula iteratively by using the scale and scheme parameters of $\alpha_{\overline{MS}}(\mu)$. Noting that $\tau_{\overline{MS}} = 2\beta_0^2\beta_1^{-1}\ln(\mu/\Lambda_{\overline{MS}}^{\underline{'H}})$, we obtain

$$\alpha_{\overline{\mathrm{MS}}}(\mu) = \frac{4\pi}{\beta_0 \ln(\mu^2 / \Lambda_{\overline{\mathrm{MS}}}^{\mathrm{'tH}^2})} \left[1 - \frac{\beta_1 \ln[\beta_0^2 \beta_1^{-1} \ln(\mu^2 / \Lambda_{\overline{\mathrm{MS}}}^{\mathrm{'tH}^2})]}{\beta_0^2 \ln(\mu^2 / \Lambda_{\overline{\mathrm{MS}}}^{\mathrm{'tH}^2})} \right] + \cdots .$$
(64)

This differs from the definition as given by the Particle Data Group [19], where $\Lambda_{\overline{MS}}$ is defined so to make the coefficient inside the double logarithm unitary:

$$\alpha_{\overline{\mathrm{MS}}}(\mu) = \frac{4\pi}{\beta_0 \ln(\mu^2 / \Lambda_{\overline{\mathrm{MS}}}^2)} \left[1 - \frac{\beta_1 \ln[\ln(\mu^2 / \Lambda_{\overline{\mathrm{MS}}}^2)]}{\beta_0^2 \ln(\mu^2 / \Lambda_{\overline{\mathrm{MS}}}^2)} \right] + \cdots .$$
(65)

The relation between $\Lambda_{\overline{MS}}$ and $\Lambda_{\overline{MS}}^{\underline{'tH}}$ can be found to be

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$$\Lambda_{\overline{\rm MS}}^{'\underline{\rm tH}} = \left[\frac{\beta_1}{\beta_0^2}\right]^{-\beta_1/2\beta_0^2} \Lambda_{\overline{\rm MS}} . \tag{66}$$

For $N_f = 5$ we have $\Lambda_{\overline{MS}}^{\underline{'H}} = 1.1477 \Lambda_{\overline{MS}}$, thus, the difference between the two definitions is small in practice.

VIII. CONCLUSIONS

To summarize, we have explained the use of extended renormalization group equations to relate physical observables. This approach provides a new and transparent interpretation of the Grunberg-Dhar-Gupta schemeinvariant method [2,8] in the language of a universal coupling function. The most distinctive feature of this formalism is that, in this approach, the perturbative series of a physical observable only serves to identify the scale and scheme parameters. The final prediction is obtained by the evolution of a universal coupling function. The prediction is scale-scheme independent in the sense that given the initial perturbative series in any scheme at any scale, we will always obtain its correct scale and scheme parameter and hence arrive at the same prediction. We have shown that this formalism sets the ground for a reliable error analysis, and that $\Lambda_{\overline{\text{MS}}}$ can be unambiguously defined as the pole in the associated 't Hooft scheme. Finally, we have shown that this formalism is equivalent to the fastest apparent convergence criterion in the absence of information on scheme parameters.

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