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Relating Physical Observables in QCD without Scale-Scheme Ambiguity*

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Abstract

We discuss the Stückelberg-Peterman extended renormalization group equations in perturbative QCD, which express the invariance of physical observables under renormalization-scale and scheme-parameter 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 beta functions. We propose the use of these evolution equations instead of 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 $\Lambda_{\overline{\rm MS}}$ as the pole in the associated 't Hooft scheme. A concrete application to $R(e^+e^- \to \text{hadrons})$ is presented.

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The scale-scheme ambiguity problem [1,2,3] remains as one of the major cornerstones 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 N-th 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:

$$R_N = r_0 \alpha_S^p(\mu) + r_1(\mu)\alpha_S^{p+1}(\mu) + \cdots + r_N(\mu)\alpha_S^{p+N}(\mu) \ . \tag{1}$$

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 [4,5] has accentuated the need for study on the scale-scheme dependence (e.g., see Ref. [6]).

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. Secondly, besides 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 criterion [2] and the BLM method [3].

In this paper we propose the use of the Extended Renormalization Group Equations as a transparent solution to 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 scheme-parameter space. This approach sets the ground for a reliable error analysis and also provides a precise definition for $\Lambda_{\overline{\rm MS}}$.

We will consider the case of QCD with N_f massless quarks. Let us first explain the concept of the universal coupling function in QCD. It is well-known that at the renormalization stage a particular subtraction prescription and a particular renormalization scale must be specified. Let us parametrize the subtraction prescription by an infinite set of continuous "scheme parameters" $\{c_i\}$ and the renormalization scale by μ. The universal coupling function (see Fig. 1) is the extension of an ordinary coupling constant to include the dependence on the scheme parameters $\{c_i\}$:

$$\alpha = \alpha(\mu/\Lambda, \{c_i\}) \ . \tag{2}$$

For the moment, the presence of the quantity Λ in the previous expression can be justified on dimensional grounds. We will identify it later with the 't Hooft scale

of the chosen scheme.

Stevenson [1] has shown that one can identify the beta-function coefficients of a renormalization scheme as its scheme parameters. That is, if a given scheme has the following beta-function expansion:

$$\beta(\alpha) = \frac{d}{d\log\mu^2}\left(\frac{\alpha}{4\pi}\right) = -\beta_0\left(\frac{\alpha}{4\pi}\right)^2 - \beta_1\left(\frac{\alpha}{4\pi}\right)^3 - \beta_2\left(\frac{\alpha}{4\pi}\right)^4 + \cdots \ ; \qquad (3)$$

then, the coefficients $\{\beta_i, \quad i = 2, 3, \ldots\}$ can be considered as the corresponding scheme parameters. (The scheme invariance of the first two coefficients β_0 and β_1 is a well-known fact. It is important not to confuse the coefficients β_i with the $\beta_{(i)}$ functions to be introduced later.) It will be very convenient to use the first two coefficients of the beta functions to rescale the coupling constant and the scale parameter $\log\mu^2$. Let us define the rescaled coupling constant and the rescaled scale parameter as

$$a = \frac{\beta_1}{\beta_0}\frac{\alpha}{4\pi} \ , \qquad \tau = \frac{2\beta_0^2}{\beta_1}\log(\mu/\Lambda) \ . \qquad (4)$$

Then, the rescaled beta function takes the canonical form:

$$\beta(a) = \frac{da}{d\tau} = -a^2(1 + a + c_2a^2 + c_3a^3 + \cdots) \ , \qquad (5)$$

with $c_n = \beta_n\beta_0^{n-1}/\beta_1^n$ for $n = 2, 3, \cdots$. This rescaling process serves to "unitarize" the expansion coefficients. For a well-behaved scheme in QCD, we would expect its beta-function expansion to roughly resemble a geometrical series, at least for the first few coefficients. In fact, for the $\overline{\rm MS}$ scheme we have $c_2^{\overline{\rm MS}} = \beta_2^{\overline{\rm MS}}\beta_0/\beta_1^2$,

where [7]

$$\begin{aligned}\beta_0 &= 11 - \frac{2}{3}N_f \ , \\ \beta_1 &= 102 - \frac{38}{3}N_f \ , \\ \beta_2^{\overline{\rm MS}} &= \frac{2857}{2} - \frac{5033}{18}N_f + \frac{325}{54}N_f^2 \ ,\end{aligned} \tag{6}$$

and for $N_f = 0, 1, 2, 3, 4, 5, 6$ we have respectively $c_2^{\overline{\rm MS}} = 1.5103, 1.4954, 1.4692, 1.4147, 1.2851, 0.92766, -0.33654$. We can clearly see that indeed $c_2^{\overline{\rm MS}}$ is of order of magnitude unity. This should be contrasted with the large value of $\beta_2^{\overline{\rm MS}}$ before the rescaling process.

The Extended Renormalization Group Equations simply express the invariance of physical quantities under scale- and scheme-parameter transformations. These equations have been studied long ago by Stückelberg and Peterman [8] and later by Stevenson [1]:

$$\begin{aligned}\frac{\delta R}{\delta \tau} &= \beta \frac{\partial R}{\partial a} + \frac{\partial R}{\partial \tau} = 0 \ , \\ \frac{\delta R}{\delta c_n} &= \beta_{(n)} \frac{\partial R}{\partial a} + \frac{\partial R}{\partial c_n} = 0 \ .\end{aligned} \tag{7}$$

Various quantities in these equations need explanation.

First of all, notice the distinction between $\delta/\delta\tau$ and $\partial/\partial\tau$. The partial derivative $\delta/\delta\tau$ takes into account the full variation of R under τ transformation, whereas the partial derivative $\partial/\partial\tau$ affects only the expansion coefficients of R. An analogous distinction holds between $\delta/\delta c_n$ and $\partial/\partial c_n$. In other words, in the left-hand side

$$R = R(\tau, \{c_i\}) \ , \tag{8}$$

whereas in the right-hand side

$$R = R(a, r_n(\tau, \{c_i\})) \ . \tag{9}$$

Mathematically these are two different functions since their domains are different. However, it is common practice to use the same notation for both and draw the difference only for their partial derivatives.

The fundamental beta function that appears in Eqs. (7) is defined as:

$$\beta(a, \{c_i\}) \equiv \frac{\delta a}{\delta \tau} = -a^2(1 + a + c_2 a^2 + c_3 a^3 + \cdots) \ , \tag{10}$$

and the extended or scheme-parameter beta functions are defined as:

$$\beta_{(n)}(a, \{c_i\}) \equiv \frac{\delta a}{\delta c_n} \ . \tag{11}$$

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

$$\frac{\delta^2 a}{\delta \tau \delta c_n} = \frac{\delta^2 a}{\delta c_n \delta \tau} \tag{12}$$

implies

$$\frac{\delta \beta_{(n)}}{\delta \tau} = \frac{\delta \beta}{\delta c_n} \ , \tag{13}$$

$$\beta \beta'_{(n)} = \beta_{(n)} \beta' - a^{n+2} \ , \tag{14}$$

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

$$\begin{aligned} \beta^{-2} \left(\frac{\beta_{(n)}}{\beta} \right)' &= -a^{n+2} \ , \\ \beta_{(n)}(a, \{c_i\}) &= -\beta(a, \{c_i\}) \int_0^a dx \frac{x^{n+2}}{\beta^2(x, \{c_i\})} \ , \end{aligned} \tag{15}$$

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

$$\beta_{(n)} \sim O(a^{n+1}) \ . \tag{16}$$

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].

The extended renormalization group equations in (7) can be put into the form:

$$\begin{aligned} \frac{\partial R}{\partial \tau} &= -\beta \frac{\partial R}{\partial a} \ , \\ \frac{\partial R}{\partial c_n} &= -\beta_{(n)} \frac{\partial R}{\partial a} \ . \end{aligned} \tag{17}$$

These equations can now be interpreted in the following manner. The left-hand sides represent the variation of the expansion coefficients of R under scale-scheme transformations. Thus, a given perturbative series can be evolved into another perturbative series, provided we know the extended beta functions on the right-hand side. In fact, in the expansion series of R as given in Eq. (1), the only quantities that cannot be modified under scale-scheme transformations are the tree-level coefficient r_0 and exponent p, since they are renormalization scale- and scheme-independent.

We can standardize a perturbative series $R = r_0 a^p + \cdots$ by defining an effective charge a_R (see Grunberg in Ref. [2]) by:

$$a_R \equiv \left(\frac{R}{r_0} \right)^{1/p} \ . \tag{18}$$

Since R, r_0 and p are all renormalization scale and scheme invariant, the effective charge a_R is also scale and scheme invariant. We only need to study the evolution of one effective charge to another. The appropriate values of r_0 and p can always be put back at the end of the analysis.

More concretely, given two perturbative series:

$$\begin{aligned} R &= r_0 a_R^p = r_0 a^p + r_1 a^{p+1} + \cdots \ , \\ R' &= r'_0 a_{R'}^{p'} = r'_0 a^{p'} + r'_1 a^{p'+1} + \cdots \ , \end{aligned} \tag{19}$$

we can evolve R into R' by following the next three steps

1) Obtain the effective charge of R

$$a_R = \left(\frac{R}{r_0}\right)^{1/p} = a + \frac{r_1}{p\ r_0} a^2 + \left(\frac{r_2}{p\ r_0} + \frac{1-p}{2\ p^2}\ \frac{r_1^2}{r_0^2}\right) a^3 + \cdots \ . \tag{20}$$

2) By using the extended renormalization group equations, we can change the perturbative coefficients of a_R and evolve it into

$$a_{R'} = a + \frac{r'_1}{p'\ r'_0} a^2 + \left(\frac{r'_2}{p'\ r'_0} + \frac{1-p'}{2\ p'^2} \frac{r'^2_1}{r'^2_0}\right) a^3 + \cdots \ . \tag{21}$$

3) Obtain R' from $a_{R'}$ by

$$R' = r'_0 a_{R'}^{p'} \ . \tag{22}$$

Hence, by using the extended renormalization group equations and by appropriately raising the power and rescaling our final result, we can evolve a given perturbative series R into any other perturbative series R'. The commutativity of second partial derivatives guarantees that the final result is independent of the path chosen for evolution.

Since the universal coupling functions $a(\tau, \{c_i\})$ covers all possible choices of scale and scheme, any effective charge a_R can be expressed in terms of it:

$$a_R = a(\tau_R, \{c_i^R\}) \ , \tag{23}$$

where τ_R and c_i^R are respectively the scale and scheme parameters of R. Notice that this is also true for multiple-scale processes: given the perturbative series of a

multiple-scale process, we can also define an effective charge associated to it, and this effective charge can then be written in terms of the universal coupling function at a particular set of values of τ and $\{c_i^R\}$.

The universal coupling function is dictated by the evolution equations:

$$\begin{aligned} \frac{\delta a}{\delta \tau} &= \beta(a, \{c_i\}) = -a^2(1 + a + c_2 a^2 + \cdots) \ , \\ \frac{\delta a}{\delta c_n} &= \beta_{(n)}(a, \{c_i\}) = -\beta(a, \{c_i\}) \int_0^a dx \frac{x^{n+2}}{\beta^2(x, \{c_i\})} \ . \end{aligned} \tag{24}$$

We shall define $a(\tau, \{c_i\})$ here with the boundary condition:

$$a(0, \{0\}) = \infty. \tag{25}$$

Notice that the above equations contain no explicit reference to QCD parameters such as the numbers of colors or the number of flavors. Therefore, aside from its infinite dimensional character, $a(\tau, \{c_i\})$ is just a mathematical function like, say, Bessel functions or any other special function. Truncation of the fundamental beta function simply corresponds to evaluating $a(\tau, \{c_i\})$ in a subspace where higher order c_i are zero. In principle, this function can be computed to arbitrary degree of precision, limited only by the truncation of the fundamental beta function.*

Notice that the 't Hooft scheme [9] defined by $a_{\prime \mathrm{tH}}(\tau) \equiv a(\tau, \{0\})$ is privileged since it is totally devoid of higher-order corrections. In fact, $a_{\prime \mathrm{tH}}(\tau)$ is exactly given by the solution of

$$\frac{1}{a_{\prime \mathrm{tH}}} + \log\left(\frac{a_{\prime \mathrm{tH}}}{1 + a_{\prime \mathrm{tH}}}\right) = \tau \ . \tag{26}$$

For any single-scale process $R(\mu)$ there exists a scale $\mu = \Lambda_R^{\prime \mathrm{tH}}$ for which the

∗ The $n!$ divergence expected for the beta function coefficients of physical effective charges can impose some theoretical limit to the achievable precision. Further discussion in this direction is beyond the scope of this paper.

scale parameter $\tau_R = 2\beta_0^2\beta_1^{-1}\log(\mu/\Lambda_R^{'\rm tH})$ vanishes. We will call $\Lambda_R^{'\rm tH}$ the 't Hooft scale[†] of the R-scheme. To understand the meaning of the 't Hooft scale, let us consider the $\overline{\rm MS}$ scheme coupling constant:

$$a_{\overline{\rm MS}}(\mu) = a\left(\frac{2\beta_0^2}{\beta_1}\log(\mu/\Lambda_{\overline{\rm MS}}^{'\rm tH}), \{c_i^{\overline{\rm MS}}\}\right) \ . \tag{27}$$

Notice that *a priori* we do not know the behavior of $a_{\overline{\rm MS}}(\mu)$ at $\mu = \Lambda_{\overline{\rm MS}}^{'\rm tH}$: it could be infinite, finite, or simply not well-defined. However, $\mu = \Lambda_{\overline{\rm MS}}^{'\rm tH}$ is the pole in the 't Hooft scheme associated[⋆] to the $\overline{\rm MS}$ scheme:

$$a_{'\rm tH-\overline{\rm MS}}(\mu) \equiv a\left(\frac{2\beta_0^2}{\beta_1}\log(\mu/\Lambda_{\overline{\rm MS}}^{'\rm tH}), \{0\}\right) \ , \tag{28}$$

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 $\Lambda_{\overline{\rm MS}}$. This cures the well-known arbitrariness in the definition of $\Lambda_{\overline{\rm MS}}$ due to the presence of higher order corrections in the $\overline{\rm MS}$ scheme.

Given two effective charges, say

$$\begin{aligned} a_{\overline{\rm MS}}(\mu) &= a\left(\frac{2\beta_0^2}{\beta_1}\log(\mu/\Lambda_{\overline{\rm MS}}^{'\rm tH}), \{c_i^{\overline{\rm MS}}\}\right) \ , \\ a_R(Q) &= a\left(\frac{2\beta_0^2}{\beta_1}\log(Q/\Lambda_R^{'\rm tH}), \{c_i^R\}\right) \ , \end{aligned} \tag{29}$$

we can expand $a_R(Q)$ in a power series of $a_{\overline{\rm MS}}(\mu)$. To this end, we can perform a

† For multiple-scale processes, the sub-manifold where the scale parameter vanishes defines the "'t Hooft surface".

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

Taylor expansion around the point

$$(\tau, \{c_i\}) = \left(\frac{2\beta_0^2}{\beta_1} \log(\mu/\Lambda_{\overline{\rm MS}}^{'\rm tH}), \{c_i^{\overline{\rm MS}}\} \right) \ , \tag{30}$$

and generate a series representation for $a_R(Q)$:

$$\begin{aligned} a_R(Q) &= a\left(\frac{2\beta_0^2}{\beta_1} \log(\mu/\Lambda_{\overline{\rm MS}}^{'\rm tH}) + \bar{\tau}, \{c_i^{\overline{\rm MS}} + \bar{c}_i\} \right) \\ &= a + \left(\frac{\delta a}{\delta \tau}\right) \bar{\tau} + \left(\frac{\delta a}{\delta c_n}\right) \bar{c}_n \\ &+ \frac{1}{2!}\left[\left(\frac{\delta^2 a}{\delta \tau^2}\right) \bar{\tau}^2 + 2\left(\frac{\delta^2 a}{\delta \tau \delta c_n}\right) \bar{\tau}\bar{c}_n + \left(\frac{\delta^2 a}{\delta c_n \delta c_m}\right) \bar{c}_n \bar{c}_m \right] \\ &+ \frac{1}{3!}\left[\left(\frac{\delta^3 a}{\delta \tau^3}\right) \bar{\tau}^3 + \cdots \right] + \cdots \ , \end{aligned} \tag{31}$$

where

$$\begin{aligned} \bar{\tau} &= \frac{2\beta_0^2}{\beta_1}\left[\log(Q/\Lambda_R^{'\rm tH}) - \log(\mu/\Lambda_{\overline{\rm MS}}^{'\rm tH}) \right] \ , \\ \bar{c}_n &= c_n^R - c_n^{\overline{\rm MS}} \ , \end{aligned} \tag{32}$$

and a and its derivatives are evaluated at the point specified in Eq. (30). To order a^4, we only need the following partial derivatives:

$$\begin{aligned} \left(\frac{\delta a}{\delta \tau}\right) &= \beta = -a^2 - a^3 - c_2 a^4 + O(a^5) \ , \\ \left(\frac{\delta a}{\delta c_2}\right) &= \beta_{(2)} = a^3 + O(a^5) \ , \\ \left(\frac{\delta a}{\delta c_3}\right) &= \beta_{(3)} = \frac{1}{2}a^4 + O(a^5) \ , \\ \left(\frac{\delta^2 a}{\delta \tau^2}\right) &= 2a^3 + 5a^4 + O(a^5) \ , \\ \left(\frac{\delta^2 a}{\delta \tau \delta c_2}\right) &= -3a^4 + O(a^5) \ , \\ \left(\frac{\delta^3 a}{\delta \tau^3}\right) &= -6a^4 + O(a^5) \ . \end{aligned} \tag{33}$$

After grouping all the terms in powers of $a = a_{\overline{\rm MS}}(\mu)$, we obtain:

$$\begin{aligned} a_R(Q) = a &- \bar{\tau} a^2 + \left(\bar{c}_2 - \bar{\tau} + \bar{\tau}^2\right) a^3 \\ &+ \left(\frac{1}{2}\bar{c}_3 - (c_2 + 3\bar{c}_2)\bar{\tau} + \frac{5}{2}\bar{\tau}^2 - \bar{\tau}^3\right) a^4 \\ &+ O(a^5) \ , \end{aligned} \tag{34}$$

where $\bar{\tau}$ and $\bar{c}_n$ are as given in Eq. (32), and $c_2 = c_2^{\overline{\rm MS}}$. Although we have used R and $\overline{\rm MS}$ schemes in the derivation of this last formula, naturally it is also valid for any other pair of effective charges. Notice the occurrence of $\bar{\tau}$ and $\bar{c}_i$ in all higher order coefficients. By using the evolution equations in (24), we are effectively performing a partial resummation of the perturbative series to all orders.

Any physical quantity R calculated perturbatively in the $\overline{\rm MS}$ scheme can be put into the above standard form. Hence, we can use Eq. (34) to identify the scale and scheme parameters of the effective charge of R. In other words, to give the numerical prediction for $R = r_0 a^p + \cdots$ we proceed to

1) compute its perturbative series in terms of the coupling constant in some scheme, say $\overline{\rm MS}$ scheme,

2) standardize the series and identify the scale and scheme parameters $(\tau_R, \{c_i^R\})$ order-by-order via Eq. (34),

3) from the knowledge of $\Lambda'^{\rm tH}_{\overline{\rm MS}}$, evolve the universal coupling function $a(\tau, \{c_i\})$ to the point $(\tau_R, \{c_i^R\})$. Put back the values of r_0 and p if necessary.

Naturally we can also go in the opposite direction and obtain $\Lambda'^{\rm tH}_{\overline{\rm MS}}$ from the experimental measurement of R. In Fig. 2 we show the various experimental and theoretical errors involved in the analysis. For the measurement of $\Lambda'^{\rm tH}_{\overline{\rm MS}}$, the input experimental error must be combined with the scheme uncertainty to give the error

estimate for $\Lambda^{'\mathrm{tH}}_{\overline{\mathrm{MS}}}$. Similarly, for the prediction of $a_R(\tau)$ the error from $\Lambda^{'\mathrm{tH}}_{\overline{\mathrm{MS}}}$ must be combined with the scheme uncertainty in order to give the prediction error.

As a concrete example, let us consider the total hadronic cross section in e^+e^- annihilation $R(Q) = R(e^+e^- \to \text{hadrons})$ recently calculated to order α^3 [4,5]. For five light-quark flavors we have

$$\begin{aligned} R(Q) &= \frac{11}{3}\left[1 + \frac{\alpha}{\pi} + 1.4092\left(\frac{\alpha}{\pi}\right)^2 - 12.8046\left(\frac{\alpha}{\pi}\right)^3\right] \\ &\equiv \frac{11}{3}\left[1 + \frac{\alpha_R(Q)}{\pi}\right] \ , \end{aligned} \tag{35}$$

where we have used $\alpha = \alpha_{\overline{\mathrm{MS}}}(Q)$ for the strong coupling constant.

By putting $R(Q)$ into the standard form of Eq. (34):

$$a_R(Q) = a + 1.1176\ a^2 - 8.05426\ a^3 \ , \tag{36}$$

where $a = a_{\overline{\mathrm{MS}}}(Q)$, we can identify

$$\bar{\tau} = -1.1176 \ , \qquad \bar{c}_2 = -10.4209 \ . \tag{37}$$

Knowing that $\bar{\tau} = 2\beta_0^2\beta_1^{-1}\log(\Lambda^{'\mathrm{tH}}_{\overline{\mathrm{MS}}}/\Lambda^{'\mathrm{tH}}_R)$ and $\bar{c}_2 = c_2^R - c_2^{\overline{\mathrm{MS}}}$, we conclude that

$$\Lambda^{'\mathrm{tH}}_R = 1.4443\ \Lambda^{'\mathrm{tH}}_{\overline{\mathrm{MS}}} \ , \qquad c_2^R = -9.4932 \ . \tag{38}$$

Experimentally [10] we have

$$r(31.6\ \mathrm{GeV}) = \frac{3}{11}R(31.6\ \mathrm{GeV}) = 1.0527 \pm 0.0050 \ , \tag{39}$$

which gives

$$a_R(31.6\ \mathrm{GeV}) = 0.0665 \pm 0.0063 \ . \tag{40}$$

We have to take into account the scheme uncertainty in addition to the experimental error in order to quote a correct error estimate for $\Lambda^{'\mathrm{tH}}_{\overline{\mathrm{MS}}}$ (see Fig. 3).

The scheme uncertainty of R can be quantified by a reasonable estimate of its next scheme parameter: c_3^R. G. B. West [11] has put an estimate $r_4 = -158.6$ for the coefficient r_4 in

$$R = 3\sum Q_f^2 \left[1 + r_1\left(\frac{\alpha}{\pi}\right) + r_2\left(\frac{\alpha}{\pi}\right)^2 + r_3\left(\frac{\alpha}{\pi}\right)^3 + r_4\left(\frac{\alpha}{\pi}\right)^4 + \cdots\right] . \qquad (41)$$

By reducing this equation into the standard form of Eq. (34), we arrive to a value $\bar{c}_3 = c_3^R - c_3^{\overline{\rm MS}} = -99.474$. Assuming $c_3^{\overline{\rm MS}}$ is of order unity, we conclude that $\left|c_3^R\right| \sim 100$. Although we have some reservation on West's estimate (see Ref. [12]), we shall nonetheless use it to illustrate our procedure. A better estimate of c_3^R will lead to a better error estimate for $\Lambda'^{\rm tH}_{\overline{\rm MS}}$.

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

The evolution in the scheme parameters are dictated by:

$$\begin{aligned} \frac{\delta a}{\delta c_2} &= \beta_{(2)} = -\beta \int_0^a dx \frac{x^4}{\beta^2} \sim a^3 + O(a^5) , \\ \frac{\delta a}{\delta c_3} &= \beta_{(3)} = -\beta \int_0^a dx \frac{x^5}{\beta^2} \sim \frac{1}{2}a^4 + O(a^5) , \end{aligned} \qquad (42)$$

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 a_0 and $a_\pm$ defined above, we follow the next steps:

1.– Generate the 't Hooft scheme coupling $a_{\prime \rm tH}$ by solving iteratively

$$a_{\prime \rm tH} = \frac{1}{\tau + \log\left(1 + 1/a_{\prime \rm tH}\right)} \ . \tag{43}$$

2.– Evolve $a_{\prime \rm tH}$ to a_0 by displacing in c_2. From (42) we have:

$$a_0 = \frac{a_{\prime \rm tH}}{\left(1 - 2\ c_2^R\ {a_{\prime \rm tH}}^2\right)^{1/2}} \ . \tag{44}$$

3.– Evolve a_0 to $a_\pm$ by displacing in c_3. From (42) we have:

$$a_\pm = \frac{a_0}{\left(1 \mp \frac{3}{2}\ c_3^R\ a_0^3\right)^{1/3}} \ . \tag{45}$$

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:

$$\begin{aligned} \Delta\tau_{\rm exp} &= (\tau_6 - \tau_2)/2 = 1.41 \ , \\ \Delta\tau_{\rm sch} &= (\tau_5 - \tau_3)/2 = 0.22 \ , \\ \Delta\tau_{\rm tot} &= (\tau_7 - \tau_1)/2 = 1.63 \ . \end{aligned} \tag{46}$$

These errors can be translated into uncertainties in $\Lambda_{\overline{\rm MS}}^{\prime \rm tH}$ since there is a one-to-one correspondence between τ and $\Lambda_{\overline{\rm MS}}^{\prime \rm tH}$. We can see that most error comes from the experimental error in a_R. We can also see that the experimental error and the scheme error are highly uncorrelated since $\Delta\tau_{\rm tot} \sim \Delta\tau_{\rm exp} + \Delta\tau_{sch}$. Numerically we obtain $\tau_1 = 10.129, \tau_4 = 11.666$ and $\tau_7 = 13.379$. Knowing that

$$\tau = \frac{2\beta_0^2}{\beta_1} \log\left(\frac{31.6\ \text{GeV}}{1.4443\ \Lambda_{\overline{\rm MS}}^{\prime \rm tH}}\right) \ , \tag{47}$$

we arrive at the following result for $\Lambda_{\overline{\rm MS}}^{\prime \rm tH}$:

$$\Lambda_{\overline{\rm MS}}^{\prime \rm tH} = 470^{+310}_{-200}\ \text{MeV} \ . \tag{48}$$

If there were no experimental error, the estimated scheme uncertainty would lead

to $\Lambda^{\prime \rm tH}_{\overline{\rm MS}} = 470^{+40}_{-30}$ MeV .[⋆]

As a second application of our formalism, we will show next how to use the experimental result of $a_R(31.6\ {\rm GeV})$ to predict other effective charges. Specifically, we will give a prediction for $a_{\overline{\rm MS}}(M_Z)$, where $M_Z = 91.173$ GeV is the mass of the Z-boson. The evolution of $a_R(31.6\ {\rm GeV})$ to $a_{\overline{\rm MS}}(M_Z)$ 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 $c_3^{\overline{\rm MS}} = \pm 1$ to estimate the scheme uncertainties in a_R and $a_{\overline{\rm MS}}$. For $a_{\overline{\rm MS}}(M_Z)$, 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 $c_2^{\overline{\rm MS}}$. 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 $\tau_{\overline{\rm MS}} = \tau_R - \bar{\tau}$ with $\bar{\tau} = 2\beta_0^2\beta_1^{-1}\left[\log(M_Z/\Lambda_{\overline{\rm MS}}) - \log(31.6\ {\rm GeV}/\Lambda_R)\right] = 4.339$, we find $\tau_{A'} = 14.468$ and $\tau_{C'} = 17.718$. From here and using $c_2^{\overline{\rm MS}} = 0.92766$ and $c_3^{\overline{\rm MS}} = 1$ in the $\overline{\rm MS}$ version of the Eqs. (44) and (45), we obtain: $a^{A'} = 0.05772$ and $a^{C'} = 0.04818$. Hence, we arrive at the prediction

$$a_{\overline{\rm MS}}(M_Z) = 0.0530 \pm 0.0048\ , \tag{49}$$

or equivalently,[†]

⋆ We have rounded off the above results. More precise values are $\Lambda^{\prime \rm tH}_{\overline{\rm MS}} = 472^{+310}_{-204}$ MeV for the case including experimental error, and $\Lambda^{\prime \rm tH}_{\overline{\rm MS}} = 472^{+35}_{-33}$ MeV for the case without experimental error.

† This value is higher than the world average $\alpha_{\overline{\rm MS}}(M_Z) = 0.1134 \pm 0.0035$ quoted in the Review of Particle Properties [13] but still consistent with other quoted values for $\alpha_{\overline{\rm MS}}(M_Z)$. For instance, $\alpha_{\overline{\rm MS}}(M_Z) = 0.118 \pm 0.008$ is obtained by OPAL [14]. The detailed analysis of consistency between the various experimental results is beyond the purpose of this paper.

$$\alpha_{\overline{\rm MS}}(M_Z) = 0.132 \pm 0.012 \ . \tag{50}$$

Let us show next that our formalism is closely related to the FAC (Fastest Apparent Convergence) 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

$$a_R(Q) = a_{\overline{\rm MS}}(\mu) - \bar{\tau} a^2_{\overline{\rm MS}}(\mu) \ , \tag{51}$$

with

$$\bar{\tau} = 2\beta_0^2\beta_1^{-1}\left[\log(Q/\Lambda_R^{'\rm tH}) - \log(\mu/\Lambda_{\overline{\rm MS}}^{'\rm tH})\right] \ , \tag{52}$$

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

$$\begin{aligned} a_R(Q) &= a\left(\frac{2\beta_0^2}{\beta_1}\log(Q/\Lambda_R^{'\rm tH}), \{0\}\right) \ , \\ a_{\overline{\rm MS}}(\mu) &= a\left(\frac{2\beta_0^2}{\beta_1}\log(\mu/\Lambda_{\overline{\rm MS}}^{'\rm tH}), \{0\}\right) \ , \end{aligned} \tag{53}$$

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

$$a_R(Q) = a_{\overline{\rm MS}}\left(\mu = \frac{\Lambda_{\overline{\rm MS}}^{'\rm tH}}{\Lambda_R^{'\rm tH}} Q\right) \ . \tag{54}$$

Hence, by setting the coefficient $\bar{\tau}$ in Eq. (51) 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 't Hooft scales, whether or not we know the scheme parameters. Thus, despite its apparent naïveness, FAC

actually constitutes a correct first step towards the elimination of scale-scheme ambiguity.

Finally let us comment on the definition of effective charges. The definition of α_R by $R \equiv r_0 \alpha_R^p$ is not the only possibility [15]. In fact, we can apply the extended renormalization group technique to the effective BLM charge [3] in the following manner. Given two physical quantities R and R' computed in a particular scheme

$$\begin{aligned} R(Q) &= r_0(Q)\alpha^p(\mu) + \left(r_{10}(Q) + r_{11}(Q,\mu)\beta_0\right)\alpha^{p+1}(\mu) + \cdots \ , \\ R'(Q') &= r'_0(Q')\alpha^{p'}(\mu') + \left(r'_{10}(Q') + r'_{11}(Q',\mu')\beta_0\right)\alpha^{p'+1}(\mu') + \cdots \ , \end{aligned} \tag{55}$$

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

$$\begin{aligned} R(Q) &= r_0(Q)\alpha^p_{R-BLM}(Q) + r_{10}(Q)\alpha^{p+1}_{R-BLM}(Q) + \cdots \ , \\ R'(Q') &= r'_0(Q')\alpha^{p'}_{R'-BLM}(Q') + r'_{10}(Q')\alpha^{p'+1}_{R'-BLM}(Q') + \cdots \ , \end{aligned} \tag{56}$$

with $\alpha_{R-BLM}(Q) = \alpha(\mu^\star)$ where $\mu^\star$ is the solution of $r_{11}(Q,\mu^\star) = 0$, and similarly $\alpha_{R'-BLM}(Q') = \alpha(\mu'^\star)$ where $\mu'^\star$ is the solution of $r'_{11}(Q',\mu'^\star) = 0$. 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. We can then apply the evolution equations to $\alpha_{R-BLM}(Q)$ and evolve it to $\alpha_{R'-BLM}(Q')$. Alternative definitions of effective charges have also been discussed in Ref. [15]. However, as we have shown in this paper any convenient choice of effective charge can be used to relate physical observables. In practice we can adhere to the definition $R \equiv r_0\alpha_R^p$ which has the advantage that r_0 and p are renormalization scale-scheme invariant quantities.

To summarize, we have explained the use of extended renormalization group equations to relate physical observables. 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 $\Lambda_{\overline{\rm MS}}$ 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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FIGURE CAPTIONS

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

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

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

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

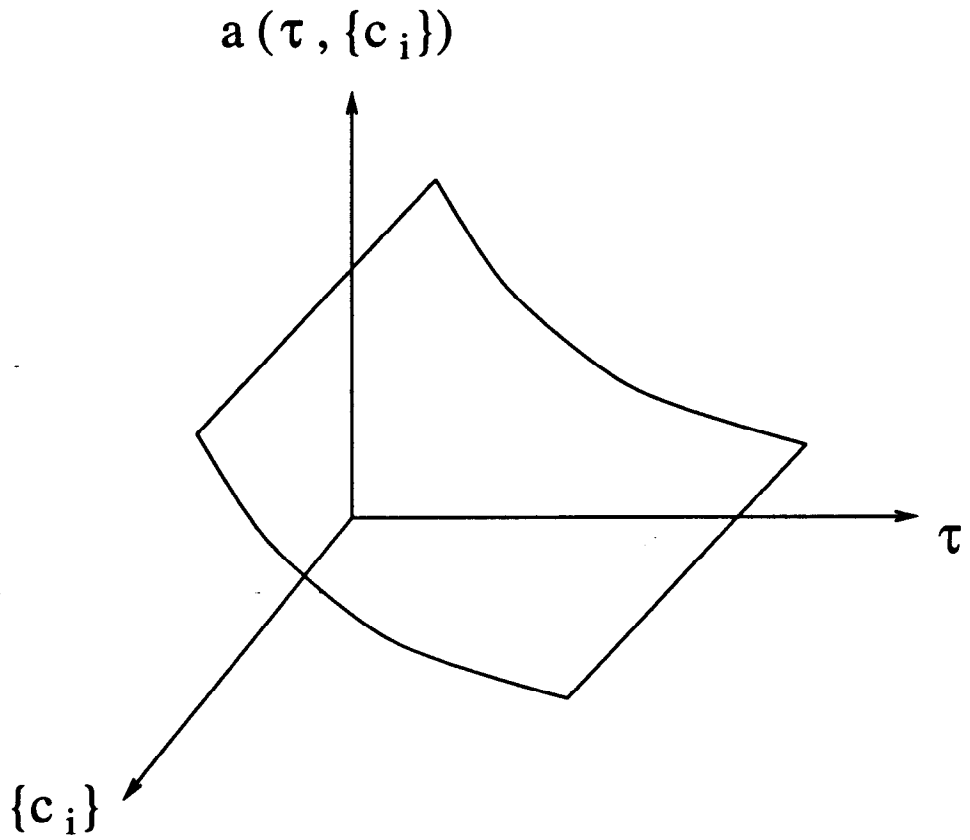

Fig. 1

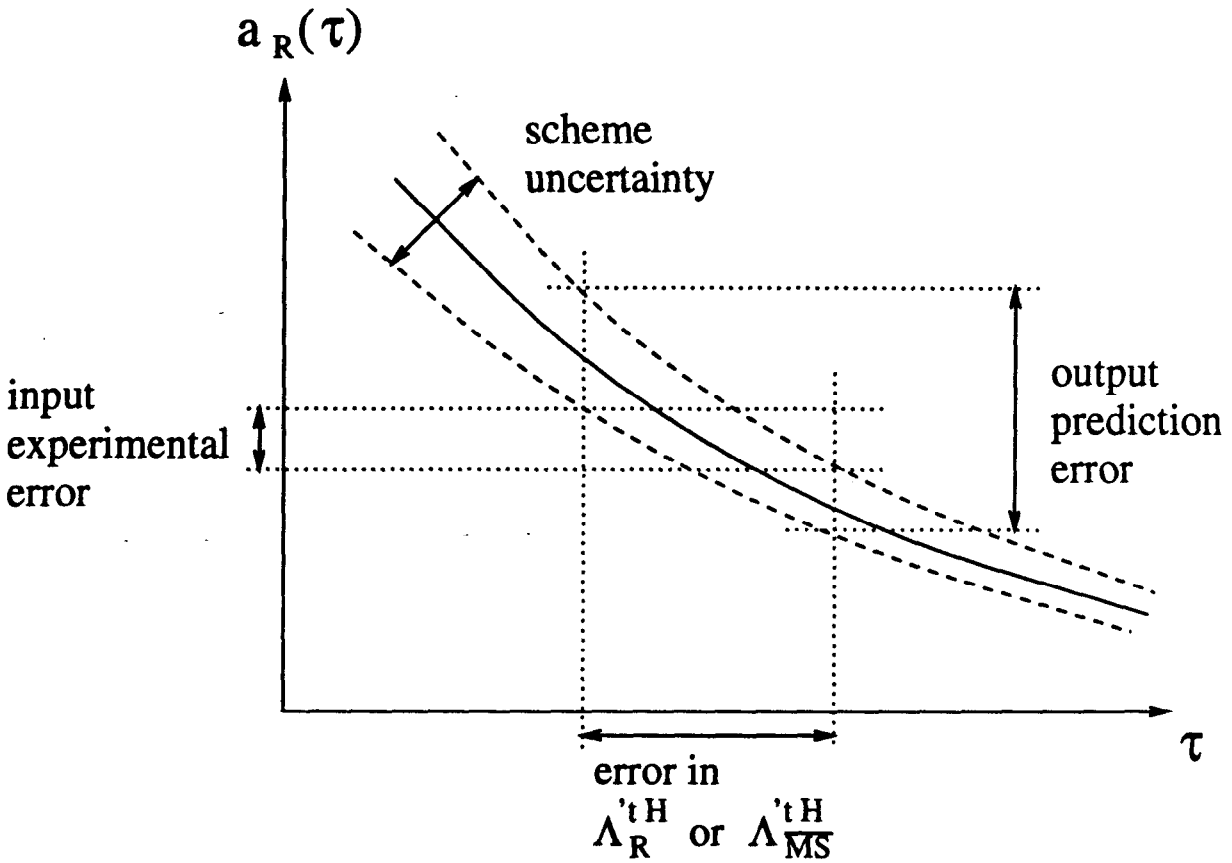
$a_R(\tau)$
scheme
uncertainty
input
experimental
error
output
prediction
error
τ
error in
$\Lambda_R^{'tH}$ or $\Lambda_{\overline{MS}}^{'tH}$

Fig. 2

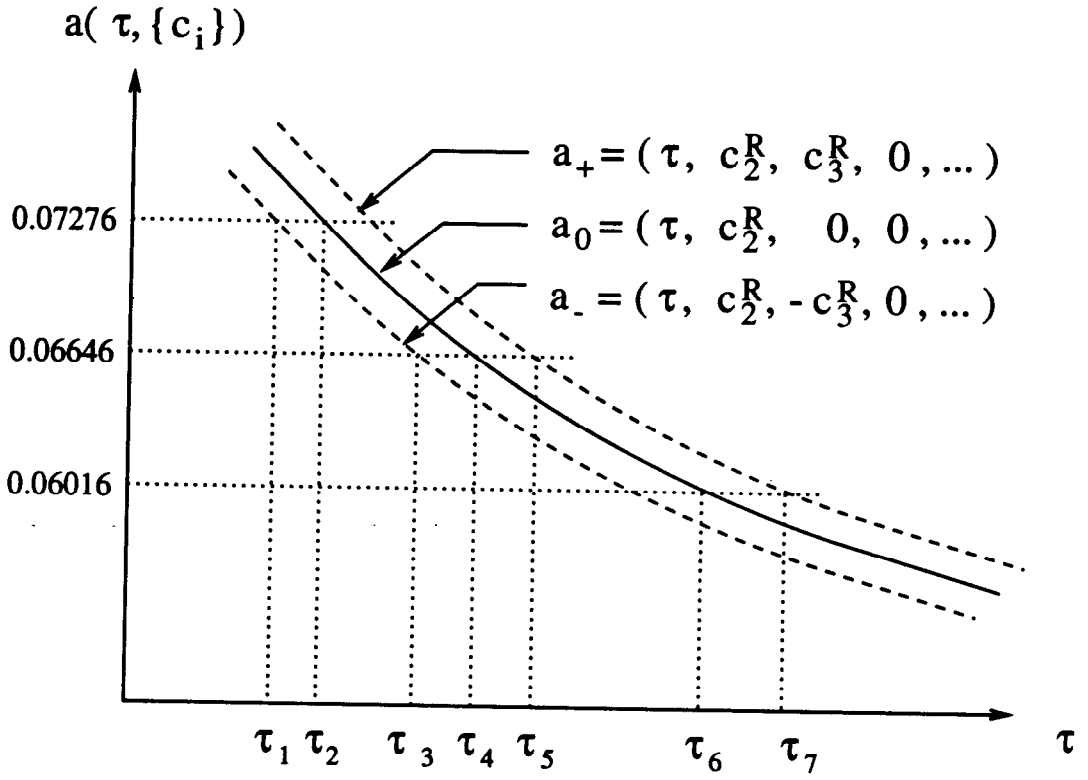
a(τ, {c_i})
a_+ = (τ, c_2^R, c_3^R, 0, ...)
a_0 = (τ, c_2^R, 0, 0, ...)
a_- = (τ, c_2^R, - c_3^R, 0, ...)
0.07276
0.06646
0.06016
τ_1 τ_2 τ_3 τ_4 τ_5 τ_6 τ_7
τ

Fig. 3

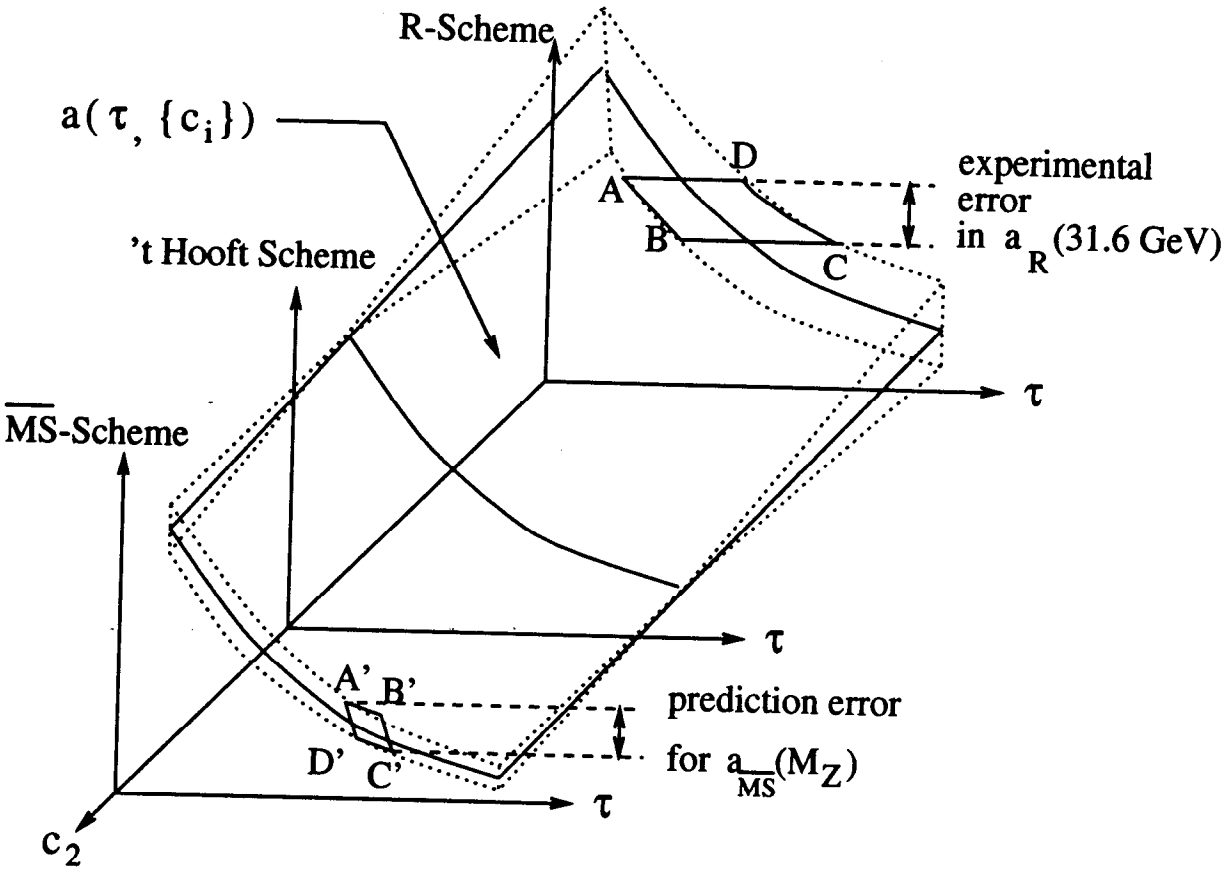
R-Scheme
a(τ, {c_i})
't Hooft Scheme
MS-Scheme
A
B
C
D
experimental
error
in a_R(31.6 GeV)
τ
τ
τ
A' B'
D' C'
prediction error
for a_MS(M_Z)
c_2

Fig. 4