

**Analysis of scheme transformations in the vicinity of an infrared fixed point**Thomas A. Rytov<sup>1</sup> and Robert Shrock<sup>2</sup><sup>1</sup>*Jefferson Physical Laboratory, Physics Department, Harvard University, Cambridge, Massachusetts 02138, USA*<sup>2</sup>*C. N. Yang Institute for Theoretical Physics Stony Brook University, Stony Brook, New York 11794, USA*

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We give a detailed analysis of the effects of scheme transformations in the vicinity of an exact or approximate infrared fixed point in an asymptotically free gauge theory with fermions. We list necessary conditions that such transformations must obey and show that, although these can easily be satisfied in the vicinity of an ultraviolet fixed point, they constitute significant restrictions on scheme transformations at an infrared fixed point. We construct acceptable scheme transformations and use these to study the scheme-dependence of an infrared fixed point, making comparison with our previous three-loop and four-loop calculations of the location of this point in the  $\overline{MS}$  scheme. We also use an illustrative hypothetical exact  $\beta$  function to investigate how accurately analyses of finite-order series expansions probe an infrared fixed point and the effect of a scheme transformation on these. Some implications of our work are discussed.

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**I. INTRODUCTION**

The evolution of an asymptotically free gauge theory from the weakly coupled ultraviolet (UV) regime to the infrared (IR) regime is of fundamental interest. Here we study this evolution for a theory with gauge group  $G$  and a given content of massless fermions. The UV to IR evolution is determined by the renormalization group  $\beta$  function of the theory, which describes the dependence of  $g \equiv g(\mu)$ , the running gauge coupling, on the Euclidean momentum scale,  $\mu$  [1]. If a theory is asymptotically free, with a small gauge coupling at a high scale  $\mu$ , and if the  $\beta$  function of this theory has a zero at a value  $\alpha_{\text{IR}}$ , then as the scale  $\mu$  decreases from large values, the coupling evolves toward  $\alpha_{\text{IR}}$ , which is thus an exact or approximate infrared fixed point (IRFP) of the renormalization group [2]. The approximate determination of the location of  $\alpha_{\text{IR}}$  from a perturbative calculation of  $\beta$  is complicated by the fact that at three-loop and higher order, the  $\beta$  function is dependent upon the scheme used for the regularization and renormalization of the theory. It is clearly important to assess the effect of this scheme dependence on the determination of  $\alpha_{\text{IR}}$ . This can be done by calculating  $\beta$  in one scheme, performing a transformation to another scheme, and comparing the respective values of  $\alpha_{\text{IR}}$  in these schemes. In Ref. [3] we pointed out that there is far less freedom in choosing scheme transformations at an IR fixed point than there is at a UV fixed point (UVFP), and we reported results from a study of scheme dependence in the calculation of an IR fixed point to three-loop and four-loop order. Since the one-loop and two-loop terms in the  $\beta$  function are scheme-independent, with scheme-dependence entering only at the level of three loops and higher, one plausibly expects that if  $\alpha_{\text{IR}}$  is small, reasonably well-behaved scheme transformations should not shift it very much, and our results confirm this expectation. However, these transformations do have a

significant effect when  $\alpha_{\text{IR}}$  is of order unity, as is generically the case when one is investigating the boundary, as a function of the number of fermions, between the infrared phases with and without spontaneous chiral symmetry breaking.

In this paper we present a detailed analysis of scheme transformations in the vicinity of an IR fixed point. We focus mainly on vectorial gauge theories but also remark on chiral gauge theories. For a vectorial gauge theory, it is straightforward to generalize our assumption of massless fermions to the case of finite-mass fermions; essentially, by use of the decoupling theorem [4], at a given scale  $\mu$ , one includes the subset of the fermions with masses small compared with  $\mu$  and integrates out those with masses greater than  $\mu$ . In contrast, for a chiral gauge theory, the gauge invariance requires massless fermions. As an input to our present work, we use our previous calculations of IR zeros of  $\beta$  to three-loop and four-loop order in the  $\overline{MS}$  scheme [5] (see also Ref. [6], the results of which agree with Ref. [5]).

We define  $\alpha = g^2/(4\pi)$ ,  $a \equiv g^2/(16\pi^2) = \alpha/(4\pi)$ , and

$$\beta_\alpha \equiv \frac{d\alpha}{dt}, \quad (1.1)$$

where  $t = \ln\mu$ . This has the series expansion

$$\beta_\alpha = -2\alpha \sum_{\ell=1}^{\infty} b_\ell a^\ell = -2\alpha \sum_{\ell=1}^{\infty} \bar{b}_\ell \alpha^\ell, \quad (1.2)$$

where  $\bar{b}_\ell = b_\ell/(4\pi)^\ell$ . The coefficients  $b_1$  and  $b_2$  were calculated in Refs. [7,8]. The  $b_\ell$  for  $\ell = 1, 2$  are independent of the scheme used for regularization and renormalization, while  $b_\ell$  with  $\ell \geq 3$  are scheme-dependent [9]. One scheme involves dimensional regularization [10] and minimal subtraction ( $MS$ ) of the poles at dimension  $d = 4$  in the resultant Euler  $\Gamma$  functions [11]. The heavily used

modified minimal subtraction ( $\overline{MS}$ ) scheme also subtracts certain related constants [12]. Calculations of  $b_3$  and  $b_4$  in the  $\overline{MS}$  scheme were given in Refs. [13,14]. Just as the calculation of  $b_1$  and demonstration that  $b_1 > 0$  was pivotal for the explanation of the approximate Bjorken scaling observed in deep inelastic electron scattering at SLAC and the development of quantum chromodynamics (QCD) [7,15], the computation of  $b_\ell$  for  $\ell = 2, 3, 4$  has been important for many QCD calculations and fits to experimental data, including data on  $\alpha_s(Q)$  [16]. Thus, although the expansion (1.2) is not a Taylor-series expansion with a finite radius of convergence, but instead is only an asymptotic series [17] and neglects nonperturbative effects such as instantons [18], comparisons of finite-order calculations with experimental data in QCD at momentum scales that are large compared with the confinement scale,  $\Lambda_{\text{QCD}} \simeq 300$  MeV, have shown that one can reliably use the perturbative  $\beta$  function in the deep Euclidean regime.

In the vicinity of the UV fixed point at  $\alpha = 0$ , one can carry out a scheme transformation that renders three- and higher-loop terms zero [19]. Below we will present an explicit construction of a scheme transformation that achieves this. Considerable work has been done on scheme (and related scale) transformations that reduce higher-order corrections in QCD calculations [20–24]. However, as we showed in Ref. [3], in order to be acceptable, a scheme transformation must satisfy a number of conditions, and although these can easily be satisfied in the vicinity of a UV fixed point, they are highly nontrivial, and are strong restrictions, in the vicinity of an IR fixed point. This is especially true when  $\alpha_{\text{IR}}$  grows to a value of order unity, so that the infrared theory is becoming strongly coupled.

## II. BACKGROUND

We first recall some relevant background. As noted above, except where otherwise indicated, we will consider a vectorial non-Abelian gauge theory. This theory has gauge group  $G$  and  $N_f$  massless (Dirac) fermions transforming according to a representation  $R$ . For a given  $G$  and  $R$ , as  $N_f$  increases,  $b_1$  decreases and eventually vanishes at [25,26]

$$N_{f,b1z} = \frac{11C_A}{4T_f}. \quad (2.1)$$

Since we restrict our considerations to an asymptotically free theory, we require that, with our sign conventions,  $b_1 > 0$ , which implies an upper limit on  $N_f$ , namely,

$$N_f < N_{f,\text{max}} \equiv N_{f,b1z}. \quad (2.2)$$

If  $N_f$  is zero or sufficiently small, then  $b_2$  has the same positive sign as  $b_1$ , so  $\beta$  has no (perturbative) IR zero for  $\alpha \neq 0$  [27]. With a sufficient increase in  $N_f$ ,  $b_2$  vanishes. This occurs at

$$N_{f,b2z} = \frac{17C_A^2}{2T_f(5C_A + 3C_f)}. \quad (2.3)$$

For  $N_f > N_{f,b2z}$ ,  $b_2$  reverses sign, becoming negative. Since  $N_{f,b2z} < N_{f,\text{max}}$ , it follows that in the interval  $I$  defined by

$$I: N_{f,b2z} < N_f < N_{f,\text{max}}, \quad (2.4)$$

the two-loop  $\beta$  function has an IR zero at  $\alpha_{\text{IR},2\ell} = -b_1/b_2$ , i.e.,

$$\alpha_{\text{IR},2\ell} = -\frac{4\pi b_1}{b_2}, \quad (2.5)$$

which is physical for  $b_2 < 0$ . Since  $b_1$  and  $b_2$  are scheme-independent, so is  $\alpha_{\text{IR},2\ell}$ . In contrast, an IR zero calculated at  $n$ -loop ( $\ell$ ) order for  $n \geq 3$  is dependent upon the scheme  $S$  used for the calculation, so we denote it here as  $\alpha_{\text{IR},n\ell,S}$ . (In Ref. [5] we denoted this simply as  $\alpha_{\text{IR},n\ell}$  since we were working there entirely in the context of the  $\overline{MS}$  scheme.) For a given gauge group  $G$  and fermion representation  $R$  (provided that  $N_f \in I$ , so that the two-loop  $\beta$  function has an IR zero),

$$\alpha_{\text{IR},2\ell} \text{ is a decreasing function of } N_f. \quad (2.6)$$

As  $N_f$  approaches  $N_{f,\text{max}}$  from below,  $b_1 \rightarrow 0^+$ , while  $b_2$  approaches a finite negative constant, so

$$\alpha_{\text{IR},2\ell} \rightarrow 0^+ \quad \text{as } N_f \nearrow N_{f,\text{max}}. \quad (2.7)$$

For  $N_f$  in the range where an IR zero of  $\beta$  exists, it plays an important role in the UV to IR evolution of the theory [8,28]. If  $\alpha_{\text{IR},2\ell}$  is large enough, then, as  $\mu$  decreases through a scale denoted  $\Lambda$ , the gauge interaction grows strong enough to produce a bilinear fermion condensate in the most attractive channel, with attendant spontaneous chiral symmetry breaking (S $\chi$ SB) and dynamical generation of effective masses for the fermions involved [29]. In a one-gluon exchange approximation to the Dyson-Schwinger equation for the fermion propagator in a vectorial gauge theory, this occurs as  $\alpha$  increases through a value  $\alpha_{\text{cr}}$  given by  $\alpha_{\text{cr}}C_f \sim O(1)$  [30,31]. Perturbative and nonperturbative corrections to this one-gluon exchange approximation have been discussed [32]. In a chiral gauge theory this fermion condensation breaks the gauge symmetry, while in the vectorial case, the most attractive channel for fermion condensation is the singlet channel, which preserves the gauge symmetry [33]. Since the fermions that have gained dynamical masses are integrated out in the low-energy effective field theory below  $\Lambda$ , the  $\beta$  function changes, and the theory flows away from the original IR fixed point, which is thus only approximate. However, if  $\alpha_{\text{IR},2\ell}$  is sufficiently small, as is the case with a large enough (AF-preserving) fermion content, then the theory evolves from the UV to the IR without

any spontaneous chiral symmetry breaking. In this case the theory has an exact IR fixed point.

For a given  $G$  and  $N_f$  (massless) fermions in a representation  $R$ , the critical value of  $N_f$  beyond which the theory flows to the IR conformal phase is denoted  $N_{f,\text{cr}}$ . As  $N_f$  increases,  $\alpha_{\text{IR},2\ell}$  decreases, and  $N_{f,\text{cr}}$  is the value at which  $\alpha_{\text{IR},2\ell}$  decreases through  $\alpha_{\text{cr}}$ . The determination of the value of  $N_{f,\text{cr}}$  for a given gauge group  $G$  and fermion representation  $R$  is of basic field-theoretic interest. In addition, this determination is important for ongoing studies of quasiconformal gauge theories. These have a gauge coupling that gets large but runs slowly over a long interval of  $\mu$  due to an approximate IR fixed point [31]. In the region of  $N_f$  slightly less than  $N_{f,\text{cr}}$ , where the theory confines but behaves in a quasiconformal manner, some insight has been gained from continuum studies of the changes in the spectrum of gauge-singlet hadrons as compared with the spectrum in a QCD-like theory [31,34,35]. Going beyond continuum studies, there has been an intensive recent program of lattice simulations to estimate  $N_{f,\text{cr}}$  and study the properties of quasiconformal gauge theories. For example, recent lattice papers on SU(3) with fermions in the fundamental representation include [36,37], and some general reviews are given in the conferences [38]. The UV to IR evolution of a chiral gauge theory and associated sequential gauge symmetry breaking are also important for dynamical approaches to fermion mass generation [39].

Since  $\alpha_{\text{IR},2\ell}$  is  $\sim O(1)$ , especially in the quasiconformal case where  $N_f \lesssim N_{f,\text{cr}}$ , there are significant corrections to the two-loop results from higher-loop terms in  $\beta$ . These motivate one to calculate these corrections to three-loop and four-loop order, and this has been done in the  $\overline{MS}$  scheme [5,6,40]. We found that, as expected if perturbative calculations are reasonably reliable, for a given  $R$  and  $N_f$  (provided that  $N_f \in I$ , so that the two-loop beta function has an IR zero), the shift in the location of the IR zero is smaller when one goes from the three-loop to the four-loop level than when one goes from the two-loop to the three-loop level. The actual direction of the shift depends on the fermion representation,  $R$ . For the fundamental (fund.) representation, we found that, for a given  $N$  and  $N_f$ ,

$$\alpha_{\text{IR},3\ell,\overline{MS}} < \alpha_{\text{IR},4\ell,\overline{MS}} < \alpha_{\text{IR},2\ell} \quad \text{for } R = \text{fund.} \quad (2.8)$$

These shifts as a function of loop order are larger for smaller  $N_f$  and get smaller as  $N_f$  approaches  $N_{f,\text{max}}$ . For example, for  $G = \text{SU}(3)$  and  $N_f = 12$ , we calculated (cf., Table III of Ref. [5])

$$\begin{aligned} \text{SU}(3), N_f = 12: \quad & \alpha_{\text{IR},2\ell} = 0.754, \\ & \alpha_{\text{IR},3\ell,\overline{MS}} = 0.435 \\ & \alpha_{\text{IR},4\ell,\overline{MS}} = 0.470, \end{aligned} \quad (2.9)$$

so the fractional shifts are

$$\begin{aligned} \text{SU}(3), N_f = 12: \quad & \frac{\alpha_{\text{IR},3\ell,\overline{MS}} - \alpha_{\text{IR},2\ell}}{\alpha_{\text{IR},2\ell}} = -0.42 \\ & \frac{\alpha_{\text{IR},4\ell,\overline{MS}} - \alpha_{\text{IR},3\ell,\overline{MS}}}{\alpha_{\text{IR},3\ell,\overline{MS}}} = +0.07, \end{aligned} \quad (2.10)$$

and the resultant ratios are

$$\begin{aligned} \text{SU}(3), N_f = 12: \quad & \frac{\alpha_{\text{IR},3\ell,\overline{MS}}}{\alpha_{\text{IR},2\ell}} = 0.58 \\ & \frac{\alpha_{\text{IR},4\ell,\overline{MS}}}{\alpha_{\text{IR},2\ell}} = 0.62 \\ & \frac{\alpha_{\text{IR},4\ell,\overline{MS}}}{\alpha_{\text{IR},3\ell,\overline{MS}}} = 1.08. \end{aligned} \quad (2.11)$$

Qualitatively similar loop comparisons apply for other values of  $N$  and  $N_f$ .

For the other (viz., adjoint and rank-2 symmetric and antisymmetric tensor) representations that we studied in Ref. [5], we also found that higher-loop values of the IR zero of  $\beta$  were generically smaller than the two-loop value, although not all parts of the inequality in (2.8) necessarily held. As examples, for  $G = \text{SU}(2)$  and fermions in the adjoint (triplet) representation,  $\alpha_{\text{IR},2\ell} = 0.628$ ,  $\alpha_{\text{IR},3\ell,\overline{MS}} = 0.459$ , and  $\alpha_{\text{IR},2\ell,\overline{MS}} = 0.450$ , while for  $G = \text{SU}(3)$  with octet fermions,  $\alpha_{\text{IR},2\ell} = 0.419$ ,  $\alpha_{\text{IR},3\ell,\overline{MS}} = 0.306$ , and  $\alpha_{\text{IR},2\ell,\overline{MS}} = 0.308$ .

Clearly, it is important to assess the scheme-dependence in these calculations of the IR zero of  $\beta$  at three-loop and four-loop level. In particular, one would like to know quantitatively how the value of the IR zero, computed at a loop level higher than two loops, changes when one changes the scheme from the  $\overline{MS}$  scheme used in Refs. [5,6] to another scheme. This information is also useful for continuum studies of the boundary, as a function of  $N_f$  (for a given  $N$  and  $R$ ), between the IR phase with chiral symmetry breaking and the chirally symmetric IR phase. We address this question here. First, we discuss general properties of a scheme transformation.

### III. SCHEME TRANSFORMATION

#### A. General

A scheme transformation can be expressed as a mapping between  $\alpha$  and  $\alpha'$ . It will be convenient to write this as

$$a = a' f(a'). \quad (3.1)$$

To keep the UV properties the same, one requires  $f(0) = 1$ . We consider functions  $f(a')$  that are analytic about  $a = a' = 0$  and hence can be expanded in the form

$$f(a') = 1 + \sum_{s=1}^{s_{\text{max}}} k_s (a')^s = 1 + \sum_{s=1}^{s_{\text{max}}} \bar{k}_s (\alpha')^s, \quad (3.2)$$

where the  $k_s$  are constants,  $\bar{k}_s = k_s / (4\pi)^s$ , and  $s_{\text{max}}$  may be finite or infinite. For  $f(a')$  functions with infinite  $s_{\text{max}}$ , our

assumption of analyticity at  $a' = a = 0$  requires that the infinite series in Eq. (3.2) converges within some nonzero radius of convergence. Given the form (3.2), it follows that the Jacobian

$$J = \frac{da}{da'} = \frac{d\alpha}{d\alpha'} \quad (3.3)$$

satisfies

$$J = 1 \quad \text{at } a = a' = 0. \quad (3.4)$$

We have

$$\beta_{\alpha'} \equiv \frac{d\alpha'}{dt} = \frac{d\alpha'}{d\alpha} \frac{d\alpha}{dt} = J^{-1} \beta_{\alpha}. \quad (3.5)$$

This has the expansion

$$\beta_{\alpha'} = -2\alpha' \sum_{\ell=1}^{\infty} b'_{\ell} (a')^{\ell} = -2\alpha' \sum_{\ell=1}^{\infty} \bar{b}'_{\ell} (\alpha')^{\ell}, \quad (3.6)$$

where  $\bar{b}'_{\ell} = b'_{\ell}/(4\pi)^{\ell}$ . Given the equality of Eqs. (3.5) and (3.6), one can solve for the  $b'_{\ell}$  in terms of the  $b_{\ell}$  and  $k_s$ . This leads to the well-known important result that [9]

$$b'_{\ell} = b_{\ell} \quad \text{for } \ell = 1, 2, \quad (3.7)$$

i.e., that the one- and two-loop terms in  $\beta$  are scheme-independent. We note that the scheme-independence of  $b_2$  assumes that  $f(a')$  is gauge-invariant. This is evident from the fact that in the momentum subtraction (MOM) scheme,  $b_2$  is actually gauge-dependent [41] and is not equal to  $b_2$  in the  $\overline{MS}$  scheme. We restrict our analysis here to gauge-invariant scheme transformations and to schemes, such as  $\overline{MS}$ , where  $b_2$  is gauge-invariant.

If there is an IR zero in the two-loop  $\beta_{\alpha}$ , at  $\alpha_{\text{IR},2\ell}$  given by (2.5), then there is also an IR zero in the two-loop  $\beta_{\alpha'}$  at the same value of  $\alpha'$ . This is consistent with the fact that, in general, (3.1) maps  $a' = -b_1/b_2$  to  $a \neq -b_1/b_2$ , since (3.1) is an exact result, whereas the equality of two-loop IR zero values holds for the truncations of  $\beta_{\alpha}$  and  $\beta_{\alpha'}$  to two-loop order. This difference is also important to remember in analyzing shifts of the location of the IR zero of  $\beta$  function. For an illustration of this, we again take  $G = \text{SU}(3)$  and  $N_f = 12$ . In Eqs. (2.9) we listed the values of  $\alpha_{\text{IR},2\ell}$  and, in the  $\overline{MS}$  scheme, the values of the three-loop and four-loop IR zeros,  $\alpha_{\text{IR},n\ell,\overline{MS}}$ ,  $n = 3, 4$ . As an example of an acceptable scheme transformation, we consider the application of the scheme transformation  $a = (1/r) \times \sinh(ra')$  to the  $\beta$  function in the  $\overline{MS}$  scheme, which will be discussed in detail in Sec. VII below. For  $r = 6$ , we find

$$\begin{aligned} S_{\text{sh},r=6}: \quad \alpha'_{\text{IR},2\ell,S_{\text{sh},r=6}} &= \alpha_{\text{IR},2\ell} = 0.754 \\ \alpha'_{\text{IR},3\ell,S_{\text{sh},r=6}} &= 0.433, \\ \alpha'_{\text{IR},4\ell,S_{\text{sh},r=6}} &= 0.467. \end{aligned} \quad (3.8)$$

Because these zeros are calculated via truncations of the  $\beta_{\alpha'}$  function to three-loop and four-loop order, respectively, they differ slightly from the result of applying the exact (infinite-order) scheme transformation in Eq. (2.9) to the IR zeros in Eq. (2.9). Thus, the transformation  $S_{\text{sh}}$ , with  $r = 6$  maps the value  $\alpha_{\text{IR},2\ell} = 0.754$  to the value 0.739, and so forth for the others in Eq. (3.8). In compact notation,

$$\begin{aligned} S_{\text{sh},r=6}: \quad (\alpha_{\text{IR},2\ell} = 0.754) &\rightarrow 0.739, \\ (\alpha_{\text{IR},3\ell,\overline{MS}} = 0.435) &\rightarrow 0.432, \\ (\alpha_{\text{IR},4\ell,\overline{MS}} = 0.470) &\rightarrow 0.466. \end{aligned} \quad (3.9)$$

Similar comments apply for other values of  $r$  with this  $S_{\text{sh}}$  scheme transformation, and for other scheme transformations. In general, for  $N_f$  values where  $\alpha_{\text{IR},2\ell}$  is not too large, so that the perturbative estimate of the IR zero of  $\beta$  is reasonably reliable, and provided that a scheme transformation is sufficiently well-behaved, the differences between  $\alpha'_{\text{IR},n\ell,S}$  calculated to  $n$ -loop order and the result of applying the exact transformation to the initial scheme (here, the  $\overline{MS}$  scheme) are small.

For a given gauge group  $G$  and fermion representation  $R$ , as  $N_f$  approaches  $N_{f,\text{max}}$  from below, since  $\alpha_{\text{IR},2\ell} \rightarrow 0$  as  $N_f$  approaches  $N_{f,\text{max}}$  from below [cf., Eq. (2.7)], it follows that, insofar as higher-order perturbative calculations of  $\beta$  are reliable, they also yield  $\alpha_{\text{IR},n\ell} \rightarrow 0$  and, after an acceptable scheme transformation, also

$$\alpha'_{\text{IR},n\ell} \rightarrow 0^+ \quad \text{as } N_f \nearrow N_{f,\text{max}}. \quad (3.10)$$

In order to assess scheme-dependence of an IR fixed point, we have calculated the relations between the  $b'_{\ell}$  and  $b_{\ell}$  for higher  $\ell$ . For example, for  $\ell = 3, 4, 5$  we obtain

$$b'_3 = b_3 + k_1 b_2 + (k_1^2 - k_2) b_1, \quad (3.11)$$

$$b'_4 = b_4 + 2k_1 b_3 + k_1^2 b_2 + (-2k_1^3 + 4k_1 k_2 - 2k_3) b_1, \quad (3.12)$$

and

$$\begin{aligned} b'_5 = b_5 + 3k_1 b_4 + (2k_1^2 + k_2) b_3 + (-k_1^3 + 3k_1 k_2 - k_3) b_2 \\ + (4k_1^4 - 11k_1^2 k_2 + 6k_1 k_3 + 4k_2^2 - 3k_4) b_1. \end{aligned} \quad (3.13)$$

We list the somewhat longer expressions for  $b'_{\ell}$  for  $\ell = 6, 7, 8$  in the Appendix. Since the  $b_{\ell}$  have been calculated only up to  $\ell = 4$ , we will only need the above results for  $b'_3$  and  $b'_4$  in our study of the effect of performing scheme transformations on the four-loop  $\beta$  functions for a non-Abelian gauge theory. However, we will use the  $b'_{\ell}$  up to  $\ell = 8$  in our study of the effect of scheme transformations on an illustrative hypothetical exact  $\beta$  function in Sec. VIII.

From the expressions for  $b'_{\ell}$  with  $3 \leq \ell \leq 8$  that we have calculated, we can discern several general structural properties. First, in the coefficients of the terms  $b_n$  entering in the expression for  $b_{\ell}$ , the sum of the subscripts of the  $k_s$ s

is equal to  $\ell - n$  with  $1 \leq n \leq \ell - 1$ , and the products of the various  $k_s$ s correspond to certain partitions of  $\ell - n$ . For example, in the expression for  $b'_4$ , the coefficient of  $b_1$  contains the term  $-2k_1^3$  corresponding to the partition (1,1,1) of  $\ell - n = 4 - 1 = 3$ , the term  $4k_1k_2$  corresponding to the partition (1,2) of 3, and the term  $-2k_3$ , corresponding to the partition 3 of 3. However, because of cancellations, in the expression for  $b'_\ell$  for even  $\ell$ , the coefficient of  $b_n$  does not contain all of the terms corresponding to the partitions of  $\ell - n$ . For example, in the expression for  $b'_2$ , there is no  $k_1b_1$  term; in the expression for  $b'_4$ , although the partitions of 2 are  $\{(1, 1), (2)\}$ , the coefficient of  $b_2$  does not contain  $k_2$ ; and in the expression for  $b'_6$ , although the partitions of 3 are  $\{(1, 1, 1), (1, 2), (3)\}$ , the coefficient of  $b_3$  does not contain  $k_1^3$  or  $k_3$ . A corollary of the structural property above is that the only  $k_s$ s that appear in the formula for  $b'_\ell$  are the  $k_s$ s with  $1 \leq s \leq \ell - 1$ .

We note that the form for  $f(a')$  in Eq. (3.2) could be generalized further so that  $f(a')$  could include a part that is finite but nonanalytic at  $a' = 0$ . An example is

$$f(a') = \left[ 1 + \sum_{s=1}^{s_{\max}} k_s (a')^s \right] [1 + \kappa e^{-\nu/a'}], \quad (3.14)$$

where  $\kappa$  and  $\nu$  are (real) constants and  $\nu > 0$ . (In this context, we recall that expressions containing terms like  $\exp(-8\pi^2/g^2)$  naturally arise in instanton calculations.) Since no terms involving  $\kappa$  occur at any finite order of a perturbative expansion of  $f(a')$  in powers of  $a'$ , our results for  $b'_\ell$  in Eqs. (3.11), (3.12), and (3.13), (A1)–(A3) continue to hold for these scheme transformations.

## B. Transformation to 't Hooft scheme at a UVFP

Given that the  $b_\ell$  for  $\ell \geq 3$  are scheme-dependent, one may ask whether it is possible to transform to a scheme in which the  $b'_\ell$  are all zero for  $\ell \geq 3$ , i.e., a scheme in which the two-loop  $\beta$  function is exact. Here and elsewhere, by the term “exact two-loop  $\beta$  function” we mean exact in the sense of Eq. (1.2), which does not include possible nonperturbative contributions, such as could be produced by instantons [18]. Near the UV fixed point at  $\alpha = 0$ , this is possible, as emphasized by 't Hooft [19]. This is commonly called the 't Hooft scheme, and we denote it as  $S_H$ . For this and other schemes, we shall also use this symbol to refer to transformation that takes one to the given target scheme; the meaning will be clear from the context.

We next present an explicit scheme transformation which, starting from a given scheme, transforms to the 't Hooft scheme. This necessarily has  $s_{\max} = \infty$ . Our key to constructing this transformation is to take advantage of the property that  $b'_\ell$  for  $\ell \geq 3$  contains only a linear term in  $k_{\ell-1}$ , so that the equation  $b'_\ell = 0$  is a linear equation for  $k_{\ell-1}$ , which can always be solved. In order to simplify the transformation, we start by setting  $k_1 = 0$ . We then solve the equation  $b'_3 = 0$  for  $k_2$ , obtaining

$$k_2 = \frac{b_3}{b_1}. \quad (3.15)$$

We then substitute these values of  $k_1$  and  $k_2$  into the equation  $b'_4 = 0$  using our expression (3.12) and solve for  $k_3$ , obtaining

$$k_3 = \frac{b_4}{2b_1}. \quad (3.16)$$

We then continue iteratively in this manner. In the next step, we substitute these values of  $k_s$ ,  $s = 1, 2, 3$ , into the expression for  $b'_5 = 0$ , using Eq. (3.13), and solve for  $k_4$ , getting

$$k_4 = \frac{b_5}{3b_1} - \frac{b_2b_4}{6b_1^2} + \frac{5b_3^2}{3b_1^2}. \quad (3.17)$$

Proceeding in this manner, we obtain

$$k_5 = \frac{b_6}{4b_1} - \frac{b_2b_5}{6b_1^2} + \frac{2b_3b_4}{b_1^2} + \frac{b_2^2b_4}{12b_1^3} - \frac{b_2b_3^2}{12b_1^3}, \quad (3.18)$$

and

$$k_6 = \frac{b_7}{5b_1} - \frac{3b_2b_6}{20b_1^2} + \frac{8b_3b_5}{5b_1^2} + \frac{11b_4^2}{20b_1^2} - \frac{4b_2b_3b_4}{5b_1^3} + \frac{b_2^2b_5}{10b_1^3} + \frac{16b_3^3}{5b_1^3} + \frac{b_2^2b_3^2}{20b_1^4} - \frac{b_2^3b_4}{20b_1^4}. \quad (3.19)$$

One can continue this procedure iteratively to calculate  $k_s$  with arbitrarily high values in  $s$ , since the equation  $b'_\ell = 0$  is a linear equation for  $k_{\ell-1}$ , which always has a solution. This yields a two-loop  $\beta$  function that is exact. We shall refer to this transformation as the  $S_H$  transformation. Although we do not claim that this is the only way to transform to the 't Hooft scheme, it is a particularly simple way to do so.

There are several salient structural features of these expressions for the  $k_s$ s. First,  $k_s$  only depends on ratios of  $b_\ell/b_1$ . Second, the  $\ell$  values that occur in the ratios  $b_\ell/b_1$  that enter into the expression for  $k_s$  have the property that in a term proportional to

$$\frac{\prod_{i=2}^{i_{\max}} b_{\ell_i}}{b_1^j}, \quad (3.20)$$

one has

$$s = \left[ \sum_{i=2}^{i_{\max}} \ell_i \right] - j, \quad (3.21)$$

where  $i_{\max}$  is determined by  $s + j$ . As a corollary, the sets of  $\ell_i$  that enter into the numerator of Eq. (3.20) arise as subsets of the partitions of  $s + j$  that exclude the integer 1. For example, in the expression for  $k_6$ , Eq. (3.19), the products of  $b_{\ell_i}$  that enter in the terms proportional to  $b_1^{-2}$  have sets of  $\ell_i$  values that are a subset of partitions of  $6 + 2 = 8$  that exclude the value 1, including (2,6), (3,5), and (4,4), corresponding to the products  $b_2b_6$ ,  $b_3b_5$ , and

$b_4^2$ . Not all of the partitions of  $s + j$  excluding 1 are represented; in the example given, the partitions of 8 excluding 1 also include (2,2,2,2), (2,2,4), and (2,3,3), but the numerators of these terms proportional to  $b_1^{-2}$  in  $k_6$  do not include  $b_2^4$ ,  $b_2^2 b_4$ , or  $b_2 b_3^2$ .

In this 't Hooft scheme with a (perturbatively) exact two-loop  $\beta$  function, if the resultant IR zero,  $\alpha_{\text{IR},2\ell}$ , is at a sufficiently small coupling to lie in the non-Abelian Coulomb phase so that the evolution into the infrared does not entail any spontaneous chiral symmetry breaking or attendant dynamical fermion mass generation, then this is an exact IR fixed point. In this case, one can take advantage of the exact solution of the differential equation represented by the two-loop  $\beta$  function in terms of a Lambert function [42]. In contrast, if the resultant IR zero,  $\alpha_{\text{IR},2\ell}$ , is greater than the critical value,  $\alpha_{\text{cr}}$  for spontaneous chiral symmetry breaking and associated bilinear fermion condensate formation, then, as  $\mu$  decreases below a scale denoted  $\Lambda$  and  $\alpha$  increases past  $\alpha_{\text{cr}}$ , this condensate formation occurs, the fermions gain dynamical masses, and one integrates them out of the low-energy effective field theory applicable below this scale. Hence, the  $\beta$  function changes to that of a pure gluonic theory, and so one cannot use the solution in terms of a Lambert function calculated for  $\mu > \Lambda$ , but instead must match this onto a different solution with  $N_f = 0$  applicable for  $\mu < \Lambda$ . This latter solution does not involve any perturbative IR zero.

### C. Necessary conditions for an acceptable scheme transformation

In order to be physically acceptable, this transformation must satisfy several conditions,  $C_i$ . For finite  $s_{\text{max}}$ , Eq. (3.1) is an algebraic equation of degree  $s_{\text{max}} + 1$  for  $\alpha'$  in terms of  $\alpha$ . We require that at least one of the  $s_{\text{max}} + 1$  roots must satisfy these conditions. For  $s_{\text{max}} = \infty$  with nonzero  $k_s$  for arbitrarily large  $s$ , the equation for  $\alpha'$  in terms of  $\alpha$  is generically transcendental, and again we require that the physically relevant solution must satisfy these conditions. These are as follows:

- (i)  $C_1$ : the scheme transformation must map a real positive  $\alpha$  to a real positive  $\alpha'$ , since a map taking  $\alpha > 0$  to  $\alpha' = 0$  would be singular, and a map taking  $\alpha > 0$  to a negative or complex  $\alpha'$  would violate the unitarity of the theory.
- (ii)  $C_2$ : the scheme transformation should not map a moderate value of  $\alpha$ , for which perturbation theory may be reliable, to a value of  $\alpha'$  that is so large that perturbation theory is unreliable.
- (iii)  $C_3$ :  $J$  should not vanish in the region of  $\alpha$  and  $\alpha'$  of interest, or else there would be a pole in Eq. (3.5).
- (iv)  $C_4$ : The existence of an IR zero of  $\beta$  is a scheme-independent property of an AF theory, depending (insofar as perturbation theory is reliable) only on the condition that  $b_2 < 0$ . Hence, a scheme

transformation must satisfy the condition that  $\beta_\alpha$  has an IR zero if and only if  $\beta_{\alpha'}$  has an IR zero.

Since one can define a transformation from  $\alpha$  to  $\alpha'$  and the inverse from  $\alpha'$  to  $\alpha$ , these conditions apply going in both directions. These four conditions can always be satisfied by scheme transformations used to study the UV fixed point and hence in applications to perturbative QCD calculations, since the gauge coupling is small (e.g.,  $\alpha_s(m_Z) = 0.118$ ), and one can choose the  $k_s$  to have appropriately small magnitudes. By continuity, it follows that among the  $s_{\text{max}} + 1$  roots of Eq. (3.1), there is always one with a real (positive)  $\alpha' \simeq \alpha$  near the UV fixed point at  $\alpha = 0$ . For small  $\alpha$ ,  $C_1$ - $C_4$  are then met. We note that, in addition to these four conditions, there may also be other related ones that must be satisfied for a given scheme transformation to be acceptable. For example, in the  $S_1$  scheme presented in Ref. [3], it is necessary that the expression  $b_2^2 - 4b_1 b_3$  in Eq. (5.3) must be nonnegative.

### IV. EXAMPLES OF SCHEME TRANSFORMATIONS ACCEPTABLE AT A UVFP BUT NOT AT AN IRFP

In Ref. [3] we pointed out that although these conditions  $C_1$ - $C_4$  can easily be satisfied by a scheme transformation applied in the vicinity of the UV fixed point at  $\alpha = \alpha' = 0$ , they are not automatically satisfied, and are a significant constraint, on a scheme transformation that one tries to apply in the vicinity of an IR fixed point. In Ref. [3] we demonstrated this with two specific examples: (i)  $\alpha = \alpha' \tanh(\alpha')$ , and (ii) a scheme transformation with  $s_{\text{max}} = 2$ ,  $k_1 = 0$ , and  $k_2 = b_3/b_1$  designed to render  $b_3' = 0$ . Here we elaborate on these, give a third example of a scheme transformation that is acceptable at a UV fixed point but not at a general IR fixed point, and discuss some issues that arise with a fourth transformation. The two pathological transformations presented in Ref. [3] are denoted, respectively, as (i) the special  $r = 4\pi$  case of the  $S_{\text{th}}$  scheme transformation and (ii) the  $S_2$  scheme transformation, discussed below in Sec. VI and IVA respectively. Our two additional examples are the  $S_3$  scheme transformation in Sec. IV B and the transformation  $S_{\text{H}}$  to the 't Hooft scheme in Sec. IV C. In the following, to avoid overly complicated notation, we will use the generic notation  $\alpha'$  for the result of the application of each scheme transformation to an initial  $\alpha$ , with it being understood that this refers to the specific transformation under consideration. Where it is necessary to clarify, we will use a subscript to identify the specific scheme  $S$  being discussed.

#### A. The $S_2$ transformation with $s_{\text{max}} = 2$ to a scheme with $b_3' = 0$

Here we elaborate on the scheme transformation discussed in Ref. [3] with  $s_{\text{max}} = 2$  that renders  $b_3' = 0$  and is acceptable at a UV fixed point, but was shown to be unacceptable at a general IR fixed point. Because  $s_{\text{max}} = 2$ , this scheme transformation depends on two

parameters,  $k_s$  with  $s = 1, 2$ . Since  $b'_3$  depends quadratically on  $k_1$  and linearly on  $k_2$ , the solution of the desired condition  $b'_3 = 0$  is simplest if one sets  $k_1 = 0$ . Then, using Eq. (3.11) and solving this equation  $b'_3 = 0$  for  $k_2$ , one finds

$$k_2 = \frac{b_3}{b_1}. \quad (4.1)$$

This scheme transformation, denoted  $S_2$ , is then

$$S_2: \quad s_{\max} = 2, \quad k_1 = 0, \quad k_2 = b_3/b_1, \quad i.e., \\ a = a' \left[ 1 + \frac{b_3}{b_1} (a')^2 \right]. \quad (4.2)$$

Applying this  $S_2$  scheme transformation to an initial scheme, one obtains

$$b'_4 = b_4. \quad (4.3)$$

It is straightforward to calculate the  $b'_\ell$  for  $\ell \geq 5$ , but we will not need them here.

By construction, at the three-loop level,  $\beta_{a'}$  in this scheme is the same as the (scheme-independent) two-loop  $\beta$  function, so the IR zero of  $\beta_{a'}$  at the three-loop level is

$$\alpha'_{\text{IR},3\ell,S_i} = \alpha'_{\text{IR},2\ell,S_i} = \alpha_{\text{IR},2\ell} = -\frac{4\pi b_1}{b_2} \\ \text{for } S_i = S_1, S_2, S_3. \quad (4.4)$$

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$$\frac{104470N^6 + 3N_f N(-26950N^4 + 4505N^2 + 99) + N_f^2(15384N^4 - 4656N^2 + 270) + 4N_f^3 N(-112N^2 + 33)}{36[34N^3 + N_f(-13N^2 + 3)]^2} > 0. \quad (4.7)$$


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For a given value of  $N$ , the determination of the range in  $N_f$  where this inequality is satisfied involves the calculation of the zeros of the numerator of (4.7), which are solutions of a cubic equation in  $N_f$ . For  $N = 2$ , these zeros occur at  $N_f = 4.27, 8.44, 55.90$ , while for  $N = 3$  they occur at  $N_f = 6.22, 12.41, 84.32$ . As before, we restrict our consideration to the interval  $I$  given by Eq. (2.4),  $N_{f,b2z} < N_f < N_{f,\max}$ , where the two-loop  $\beta$  function has an IR zero. For  $N = 2$ , this interval  $I$  is  $5.55 < N_f < 11$ , and in this interval the inequality is violated for  $5.55 < N_f < 8.44$  and is satisfied for  $8.44 < N_f < 11$ . For  $N = 3$ , the interval  $I$  is  $8.05 < N_f < 16.5$ , and in this interval, the inequality is violated for  $8.05 < N_f < 12.41$  and is satisfied for  $12.41 < N_f < 16.5$ . For the physical, integer values of  $N_f$ , these statements are evident from the values of  $\bar{b}_\ell$  listed in Table III

of our Ref. [5]. For example, for  $N = 3$  and  $N_f = 10$ , where  $\alpha_{\text{IR},2\ell} = 2.21$ , the values of these coefficients are  $\bar{b}_1 = 0.345$ ,  $\bar{b}_2 = -0.156$ , and  $\bar{b}_3 = -0.386$ , so that

$$1 + \frac{\bar{b}_1 \bar{b}_3}{\bar{b}_2^2} = 1 + \frac{b_1 b_3}{b_2^2} = -4.47 \quad (4.8)$$

for  $G = \text{SU}(3)$ ,  $N_f = 10$ ,  $R = \text{fund}$ .

(We write this in a general form, since it holds not just for the present  $S_2$  scheme transformation, but also for the  $S_3$  and  $S_1$  transformations to be discussed below.) At the four-loop level in this  $S_2$  scheme, the IR zero is determined by the physical (smallest positive) solution of the cubic equation

$$b_1 + b_2 a' + b'_4 (a')^3 = 0. \quad (4.5)$$

In order that this transformation obey condition  $C_1$ , that it maps  $a' > 0$  to  $a > 0$ , we require that  $1 + (b_3/b_1)(a')^2 > 0$ . This inequality must be satisfied, in particular, in the vicinity of the two-loop IR zero of  $\beta$ , so substituting the (scheme-independent)  $\alpha_{\text{IR},2\ell} = \alpha'_{\text{IR},2\ell} = -b_1/b_2$  from Eq. (2.5), we obtain the inequality

$$1 + \frac{b_1 b_3}{b_2^2} > 0. \quad (4.6)$$

But, as noted in Ref. [3], this inequality is not, in general, satisfied. For example, let us consider the class of theories with  $G = \text{SU}(N)$  and  $N_f$  fermions in the fundamental representation. Substituting the scheme-independent expressions for  $b_1$  and  $b_2$  [7,8], together with the expression for  $b_3$  in the  $\overline{MS}$  scheme [13] for this class of theories, the inequality (4.6) becomes

The values of  $1 + (b_1 b_3/b_2^2)$  for  $N = 3$  and some larger values of  $N_f$  are as follows:  $-1.43$  for  $N_f = 11$  and  $-0.270$  for  $N_f = 12$ , with positive values for  $N_f \geq 13$  in the interval  $I$ , including the value  $+0.293$  for  $N_f = 13$ .

The pathology that this  $S_2$  scheme transformation violates conditions  $C_1$  and  $C_4$  is reflected in the results that one gets by actually applying it to the four-loop  $\beta$  function in the  $\overline{MS}$  scheme and solving for the IR zeros. As above, we focus on the case of fermions in the fundamental representation, with  $N_f \in I$ . We list the values of  $\alpha'_{\text{IR},3\ell,S_2}$  and  $\alpha'_{\text{IR},4\ell,S_2}$  in Table I. The three-loop values are given by Eq. (4.4). As regards the four-loop values, we find that, except for  $N_f$  value(s) near  $N_{f,\max}$ , at the upper end of the non-Abelian Coulomb phase, the cubic equation (4.5) yields a negative root and a complex-conjugate pair of roots, none of which is physically acceptable. For example, for  $N = 2$ , there is no physical root (denoted as n.p. in the table) for  $N_f \in I$  except for the highest value of  $N_f$  below  $N_{f,\max}$ , namely  $N_f = 10$ . Similarly, when  $N = 3$ , a physical root of the cubic equation first appears for  $N_f = 14$  and when  $N = 4$ , this happens when  $N_f = 19$ .

Thus, although this  $S_2$  scheme transformation is acceptable at the UV fixed point at  $\alpha = 0$  and at a sufficiently

TABLE I. Values of the IR zeros of  $\beta_\alpha$  in the  $\overline{MS}$  scheme and the respective  $\beta_{\alpha'}$  functions obtained by applying the  $S_1$ ,  $S_2$ , and  $S_3$  scheme transformations to the  $\overline{MS}$   $\beta_\alpha$  function. The listings are for an  $SU(N)$  gauge theory with  $N_f$  (massless) fermions in the fundamental representation, for  $N = 2, 3, 4$ , calculated to  $n$ -loop order and denoted as  $\alpha_{\text{IR},n\ell,\overline{MS}}$  and  $\alpha'_{\text{IR},n\ell,S_i}$ , where  $i = 1, 2, 3$ , respectively. Here,  $\alpha_{\text{IR},2\ell,\overline{MS}} = \alpha'_{\text{IR},2\ell,S_i}$  is scheme-independent, so we denote it simply as  $\alpha_{\text{IR},2\ell}$ . Since all of these  $S_i$  scheme transformations with  $i = 1, 2, 3$  yield  $b'_3 = 0$ , it follows that  $\alpha'_{\text{IR},3\ell,S_i} = \alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell}$ . The notation n.p. means not physical, i.e., there is no physical solution for  $\alpha'_{\text{IR},4\ell,S_i}$ . See text for further details.

| $N$ | $N_f$ | $\alpha_{\text{IR},2\ell}$ | $\alpha_{\text{IR},3\ell,\overline{MS}}$ | $\alpha_{\text{IR},4\ell,\overline{MS}}$ | $\alpha'_{\text{IR},4\ell,S_1}$ | $\alpha'_{\text{IR},4\ell,S_2}$ | $\alpha'_{\text{IR},4\ell,S_3}$ |
|-----|-------|----------------------------|--|--|---------------------------------|---------------------------------|---------------------------------|
| 2   | 7     | 2.83                       | 1.05                                     | 1.21                                     | 0.640                           | n.p.                            | 0.488                           |
| 2   | 8     | 1.26                       | 0.688                                    | 0.760                                    | 0.405                           | n.p.                            | 0.633                           |
| 2   | 9     | 0.595                      | 0.418                                    | 0.444                                    | 0.2385                          | n.p.                            | 0.730                           |
| 2   | 10    | 0.231                      | 0.196                                    | 0.200                                    | 0.109                           | 0.240                           | 0.248                           |
| 3   | 10    | 2.21                       | 0.764                                    | 0.815                                    | 0.463                           | n.p.                            | 0.316                           |
| 3   | 11    | 1.23                       | 0.578                                    | 0.626                                    | 0.344                           | n.p.                            | 0.391                           |
| 3   | 12    | 0.754                      | 0.435                                    | 0.470                                    | 0.254                           | n.p.                            | 0.444                           |
| 3   | 13    | 0.468                      | 0.317                                    | 0.337                                    | 0.181                           | n.p.                            | 0.4385                          |
| 3   | 14    | 0.278                      | 0.215                                    | 0.224                                    | 0.121                           | 0.321                           | 0.358                           |
| 3   | 15    | 0.143                      | 0.123                                    | 0.126                                    | 0.068                           | 0.148                           | 0.152                           |
| 3   | 16    | 0.042                      | 0.040                                    | 0.040                                    | 0.0215                          | 0.042                           | 0.042                           |
| 4   | 13    | 1.85                       | 0.604                                    | 0.628                                    | 0.365                           | n.p.                            | 0.228                           |
| 4   | 14    | 1.16                       | 0.489                                    | 0.521                                    | 0.293                           | n.p.                            | 0.276                           |
| 4   | 15    | 0.783                      | 0.397                                    | 0.428                                    | 0.235                           | n.p.                            | 0.311                           |
| 4   | 16    | 0.546                      | 0.320                                    | 0.345                                    | 0.187                           | n.p.                            | 0.339                           |
| 4   | 17    | 0.384                      | 0.254                                    | 0.271                                    | 0.146                           | n.p.                            | 0.362                           |
| 4   | 18    | 0.266                      | 0.194                                    | 0.205                                    | 0.110                           | n.p.                            | n.p.                            |
| 4   | 19    | 0.175                      | 0.140                                    | 0.145                                    | 0.0785                          | 0.193                           | 0.208                           |
| 4   | 20    | 0.105                      | 0.091                                    | 0.092                                    | 0.050                           | 0.108                           | 0.111                           |
| 4   | 21    | 0.047                      | 0.044                                    | 0.044                                    | 0.023                           | 0.048                           | 0.048                           |

weakly coupled IR fixed point at the upper end of the non-Abelian Coulomb phase, it is not acceptable at a general IR fixed point, since it fails to satisfy condition  $C_1$ . The latter pathology occurs when  $\alpha_{\text{IR}}$  grows to a value of order unity. According to the results of several lattice groups [36], for  $N = 3$ , the theory with  $N_f = 12$ , and hence also the theory with  $N_f = 13$ , evolve into the infrared in a conformal, non-Abelian Coulomb phase (other lattice groups differ on the  $N_f = 12$  case [37]). Provided that one accepts that  $N_f = 12$ , and hence also  $N_f = 13$ , are in the non-Abelian Coulomb phase, our results above show that a scheme transformation may fail to be acceptable not only at an IR fixed point in the phase with confinement and spontaneous chiral symmetry breaking (which is approximate), but also at an exact IR fixed point in the lower part of the chirally symmetric conformal phase.

### B. The $S_3$ transformation with $s_{\text{max}} = 2$ to a scheme with $b'_3 = 0$

Here we present a scheme transformation with  $s_{\text{max}} = 2$  that is also designed to render  $b'_3 = 0$  and is acceptable at a UV fixed point, but we show that it is not acceptable at a general IR fixed point. The property that  $s_{\text{max}} = 2$  and the goal of rendering  $b'_3 = 0$  are the same as those of the

transformation given in Ref. [3] (denoted  $S_2$  here). Since one uses a scheme transformation with  $s_{\text{max}} = 2$  and since  $b'_3$  depends only on  $k_1$  and  $k_2$ , it follows that a natural first choice is to try  $k_1 = 0$  and  $k_2 \neq 0$ . This was the ( $S_2$ ) transformation that was shown to be unacceptable at a general IR fixed point in Ref. [3]. Another natural choice is to set  $k_2 = k_1^2$ , since this renders the coefficient of the  $b_1$  term in  $b'_3$ , namely  $(k_1^2 - k_2)$ , equal to zero. Hence, this choice considerably simplifies the equation  $b'_3 = 0$ , which is reduced to a linear equation for  $k_1$ , with solution  $k_1 = -b_3/b_2$ . We denote this scheme transformation as  $S_3$ ,

$$S_3: s_{\text{max}} = 2, \quad k_1 = -\frac{b_3}{b_2}, \quad k_2 = k_1^2 = \frac{b_3^2}{b_2^2}, \quad (4.9)$$

and study it here. As before, we also use  $S_3$  to refer to the scheme that is obtained by applying this transformation to an initial scheme such as the  $\overline{MS}$  scheme. We denote the resultant IR zero of  $\beta_{\alpha'}$  at the  $n$ -loop level as  $\alpha'_{\text{IR},n\ell,S_3}$ . Evaluating Eq. (3.12) for  $b'_4$  in this scheme, we calculate

$$b'_4 = b_4 - \frac{b_3^2}{b_2} - \frac{2b_1b_3^3}{b_2^3} \quad \text{for } S_3. \quad (4.10)$$

The function  $f(a')$  takes the simple form



$$f(a') = 1 + \xi + \xi^2 \quad \text{for } S_2,$$

$$\text{where } \xi \equiv k_1 a' = -\frac{b_3 a'}{b_2}. \quad (4.11)$$

Now  $1 + \xi + \xi^2$  is always positive, with no real zero in  $\xi$  (and a minimum at  $\xi = -1/2$ , where this polynomial is equal to  $3/4$ ). The Jacobian for this transformation is

$$J = 1 + 2\xi + 3\xi^2 \quad \text{for } S_3. \quad (4.12)$$

This  $J$  is also positive, with no real zero in  $\xi$  (and a minimum at  $\xi = -1/3$ , where  $J = 2/3$ ). As with the  $S_2$  scheme, at the three-loop level,  $\beta_{a'}$  in this scheme is the same as the two-loop  $\beta$  function, so the IR zero of  $\beta_{a'}$  at the three-loop level satisfies Eq. (4.4). At the four-loop level in this  $S_3$  scheme, the IR zero is determined by the physical (smallest positive) solution of the cubic equation (4.5) with  $b'_4$  given by Eq. (4.10).

We have calculated the resultant  $\alpha'_{\text{IR},n\ell} \equiv \alpha_{\text{IR},n\ell,S_3}$  in this  $S_3$  scheme up to the ( $n = 4$ )-loop level. In Table I we list values of the  $n$ -loop IR zero,  $\alpha'_{\text{IR},n\ell,S_3}$  for  $n = 2, 3, 4$  for relevant  $N_f$ , with fermions in the fundamental representation and several values of  $N$ . For comparison we also include the values of  $\alpha_{\text{IR},n\ell,\overline{MS}}$  for  $n = 3, 4$  in the  $\overline{MS}$  scheme from Ref. [5]. Since the two-loop value is scheme-independent, we denote it simply as  $\alpha_{\text{IR},2\ell}$ . The relation (4.4) is reflected in the entries in the table. The four-loop zero is denoted as  $\alpha'_{\text{IR},4\ell,S_3}$ . In contrast with  $\alpha_{\text{IR},n\ell,\overline{MS}}$  and  $\alpha'_{\text{IR},n\ell,S_1}$ , which decrease monotonically as a function of  $N_f$  for a given  $N$ ,  $\alpha'_{\text{IR},4\ell,S_3}$  behaves non-monotonically as a function of  $N_f$ , first increasing and then decreasing.

But our overriding result here is that the  $S_3$  scheme transformation does not yield any physical value for  $\alpha'_{\text{IR},4\ell,S_3}$  in the case of SU(4) with  $N_f = 18$  in the fundamental representation. In this case, the above-mentioned cubic equation has only a negative root and a complex-conjugate pair of roots. Hence, this  $S_3$  scheme transformation fails conditions  $C_1$  and  $C_4$  and must be rejected as unacceptable in the vicinity of a general IR fixed point. This theory with an SU(4) gauge group and  $N_f = 18$  fermions is likely to be in a non-Abelian Coulomb phase in the infrared. Assuming this is the case, this provides another example of how a scheme transformation can be pathological not just in the confined phase with spontaneous chiral symmetry breaking, but also in the infrared conformal phase.

### C. The $S_H$ transformation to the 't Hooft scheme

In Sec. III B we have constructed a scheme transformation that can be applied to an arbitrary initial scheme to shift to the 't Hooft scheme, with  $b'_\ell = 0$  for  $\ell \geq 3$  and thus a (perturbatively) exact two-loop  $\beta$  function. By the general continuity arguments that we have presented, this

scheme transformation satisfies all of the requisite conditions to be an acceptable transformation in the vicinity of the UV fixed point at  $\alpha = \alpha' = 0$ . However, one encounters a complication with this transformation at an IR fixed point. This can be explained as follows. For a given group  $G$  and fermion representation  $R$ , as  $N_f$  increases toward  $N_{f,\text{max}}$ ,  $b_1 \rightarrow 0$ , while  $b_2$  and, in the initial scheme, the  $b_\ell$  with  $\ell \geq 3$ , approach finite nonzero values. Hence, since the coefficient  $k_s$  is a sum of terms each of which contains an inverse power of  $b_1$ , it follows that, as  $N_f$  takes on values close to  $N_{f,\text{max}}$ , these  $k_s$  coefficients may have arbitrarily large magnitudes as  $s \rightarrow \infty$ . For a particular term  $k_s(a')^s$  in the sum (3.2), much of this growth is cancelled, since,  $a'_{\text{IR},2\ell} \propto b_1$ . However, since one must use an infinite number of  $k_s$  terms to render all of the  $b'_\ell$  equal to zero for this  $S_H$  transformation, one encounters the issue of the convergence of the infinite series for  $f(a')$  in Eq. (3.2). Note that this is not an issue of strong coupling, as are the pathologies in the  $S_2$ ,  $S_3$ , and  $S_{\text{th}}$  scheme transformations; it occurs in the weakly coupled, non-Abelian Coulomb phase. We do not claim here that it is impossible to construct an acceptable scheme transformation to get to the 't Hooft scheme in the vicinity of an IR fixed point, only that one encounters delicate issues of convergence with the  $S_H$  scheme, since for a fixed  $N_f$  near to  $N_{f,\text{max}}$ , the  $k_s$  may have unbounded magnitudes as  $s \rightarrow \infty$ .

As we will discuss below, the scheme transformation  $S_1$  contains a parameter (denoted  $k_{1p}$ ) that also grows large as  $N_f$  approaches  $N_{f,\text{max}}$ , but, although inconvenient, this is much less serious, since there is only a single parameter involved, since  $s_{\text{max}} = 1$ , not an infinite number, as with the  $S_H$  transformation, and the growth of this single parameter, restricted to integer values of  $N_f$ , is bounded.

## V. THE TRANSFORMATION $S_1$ WITH $s_{\text{max}} = 1$ TO A SCHEME WITH $b'_3 = 0$

We next proceed to construct and study scheme transformations that are acceptable at an (exact or approximate) IR fixed point and use them to study the scheme dependence of the location of this fixed point. For comparative purposes, it is useful to begin by discussing the scheme denoted  $S_1$  that we presented in Ref. [3], on which we will give more details here.

The original motivation for our construction of this  $S_1$  scheme transformation was the idea of designing a transformation that would render at least one of the  $b'_\ell$  with  $\ell \geq 3$  equal to zero, namely  $b'_3$ . In turn, this was motivated by the idea of having a scheme transformation that achieves at least one step in the sequence of steps that defines a transformation to the 't Hooft scheme, where  $b'_\ell = 0$  for all  $\ell \geq 3$ . The next steps in this direction would be to design a scheme transformation that would render both  $b'_3 = 0$  and  $b'_4 = 0$  at an IR fixed point, and then one that would render  $b'_\ell = 0$  for  $\ell = 3, 4, 5$ , and so forth, up to

a fixed value of  $s$ . As a reasonable first exploration of such endeavors, we opted to focus on scheme transformations that rendered just  $b'_3 = 0$ . We have considered three of these, labelled  $S_j$ ,  $j = 1, 2, 3$ , and shown that the  $S_2$  and  $S_3$  transformations are not acceptable at a general IR fixed point. As we will show below, the  $S_1$  scheme transformation has the inconvenient feature that the  $k_s$  coefficients grow as one approaches the upper end of the non-Abelian Coulomb phase, producing a rather strong scheme-dependence even at the four-loop level. This  $S_1$  scheme transformation is, nevertheless, valuable as a lesson that shows how large scheme-dependent effects can be. As we will show below in Sec. (7.1), the  $S_{\text{shr}}$  scheme transformation in Eq. (7.1) with moderate values of  $r$  is better-behaved and, when applied to the  $\beta$  function in the  $\overline{MS}$  scheme, produces smaller shifts in the location of the IR zero than the  $S_1$  transformation.

We proceed to the details of the construction of the  $S_1$  scheme transformation presented in Ref. [3]. We assume  $N_f \in I$ , so a two-loop IR zero of  $\beta$  exists. Since  $s_{\text{max}} = 1$ , Eq. (3.1) reads  $a = a'(1 + k_1 a')$ . Although this quadratic equation has two formal solutions, only the solution

$$\alpha'_+ = \frac{1}{2\bar{k}_1} \left( -1 + \sqrt{1 + 4\bar{k}_1 \alpha} \right), \quad (5.1)$$

is acceptable, since only this solution has  $\alpha \rightarrow \alpha'$  as  $\alpha \rightarrow 0$ .

This scheme transformation was designed to render  $b'_3 = 0$ , so the next step is to solve the equation  $b'_3 = 0$  using Eq. (3.11), viz.,

$$b_3 + k_1 b_2 + k_1^2 b_1 = 0, \quad (5.2)$$

for the parameter  $k_1$ . Formally, Eq. (5.2) has two solutions,

$$k_{1p}, \quad k_{1m} = \frac{1}{2b_1} \left[ -b_2 \pm \sqrt{b_2^2 - 4b_1 b_3} \right], \quad (5.3)$$

where  $(p, m)$  refer to  $\pm$ . We will focus on  $G = \text{SU}(N)$  with fermions in the fundamental and adjoint representation. Of the two formal solutions in Eq. (5.3), only  $k_{1p}$  is allowed. To show this, we consider  $k_{1m}$ . We must be able to use this for  $N_f \in I$ , including the lower end of this interval, where  $N_f$  approaches  $N_{f,b2z}$  from above. Precisely at the lower end, as  $N_f \searrow N_{f,b2z}$ ,  $b_2 \rightarrow 0^-$  and  $\alpha_{\text{IR},2\ell} \rightarrow \infty$ , so clearly one cannot trust perturbative calculations at or near this point. However, we will at least require that the transformation should obey the conditions  $C_1$ - $C_4$  for  $N_f \geq N_{f,b2z}$  where  $\alpha_{\text{IR},2\ell}$  is not too large. As shown in Ref. [5], in this region of  $N_f$ ,  $b_3 < 0$ , so that, taking into account that both  $b_2$  and  $b_3$  are negative in this region, we can reexpress  $k_{1m}$  as

$$k_{1m} = \frac{1}{2b_1} \left[ |b_2| - \sqrt{b_2^2 + 4b_1 |b_3|} \right] \quad \text{for } N_f \geq N_{f,b2z}. \quad (5.4)$$

As  $N_f \searrow N_{f,b2z}$ ,  $b_2 \rightarrow 0^-$ , so  $k_{1m} \rightarrow -\sqrt{|b_3|/|b_1|}$ . Substituting this into Eq. (5.1), using  $\bar{k}_1 = k_1/(4\pi)$ , we have

$$\begin{aligned} \alpha'_+ &= \frac{1}{2\bar{k}_{1m}} \left( -1 + \sqrt{1 + 4\bar{k}_{1m} \alpha} \right) \\ &= \frac{1}{2|\bar{k}_{1m}|} \left( 1 - \sqrt{1 - 4|\bar{k}_{1m}| \alpha} \right). \end{aligned} \quad (5.5)$$

Next, substituting the value of  $\alpha_{\text{IR},2\ell}$  from Eq. (2.5) as a relevant estimate, the square root in Eq. (5.1) becomes

$$\left[ 1 - \frac{\sqrt{|b_1| |b_3|}}{|b_2|} \right]^{1/2}. \quad (5.6)$$

As  $N_f$  approaches  $N_{f,b2z}$  from above and  $b_2 \rightarrow 0^-$ , the expression in this square root becomes negative, so that the square root itself is imaginary. Hence, if one were to try to use  $k_{1m}$  with this scheme transformation, then a real  $\alpha \approx \alpha_{\text{IR},2\ell}$  would get mapped via Eq. (5.1) to a complex, unphysical  $\alpha'$ , clearly violating conditions  $C_1$ ,  $C_2$ , and  $C_4$ . We therefore cannot use the  $k_{1m}$  solution in Eq. (5.3) but must instead choose the  $k_{1p}$  solution. We next show that the discriminant in the expression for  $k_{1p}$  in Eq. (5.3),  $D_k = b_2^2 - 4b_1 b_3$ , is nonnegative (actually positive), as it must be. This property follows because  $b_3 < 0$  in this interval for the representations under consideration, since  $N_{f,b3z} < N_{f,b2z}$  (where we use the relevant solution of the quadratic equation, labelled  $N_{f,b3z,-}$  in Eq. (3.16) of our Ref. [5]). Hence, we can write  $D_k = b_2^2 + 4b_1 |b_3| > 0$ . We denote the present scheme transformation with this choice as  $S_1$ :

$$S_1: s_{\text{max}} = 1, \quad k_1 = k_{1p}, \quad \text{i.e.,} \quad a = a'(1 + k_{1p} a'). \quad (5.7)$$

Physically,  $N_f$  is restricted to take on nonnegative, integral values. However, since in much of our analysis, we do consider the formal analytic continuation of  $N_f$  from these integral values to positive real numbers, we remark on one effect of this continuation here. For a given gauge group  $G$  and fermion representation  $R$ , if one carries out this analytic continuation and considers the formal limit  $N_f \nearrow N_{f,\text{max}}$ , i.e., as one approaches the upper end of the non-Abelian Coulomb phase, as a function of  $N_f$ , since  $b_1 \rightarrow 0$ ,  $k_{1p}$  diverges because of the prefactor  $(2b_1)^{-1}$  in Eq. (5.3). This divergence in  $k_{1p}$  is cancelled in the actual  $S_1$  transformation, which still maps  $\alpha_{\text{IR},2\ell} \rightarrow 0$  to  $\alpha' \rightarrow 0$  as  $N_f \nearrow N_{f,\text{max}}$ . This can be seen by expanding Eq. (5.1):  $\alpha'_+ \rightarrow \sqrt{\alpha/\bar{k}_{1p}} \rightarrow 0$ . Although one does not have to worry about this if one restricts  $N_f$  to physical, integer values in the asymptotically free interval  $N_f < N_{f,\text{max}}$ , it does lead to significant residual scheme dependence in the comparison between the four-loop IR zero in the  $\overline{MS}$  scheme, and the four-loop zero computed by applying this  $S_1$  scheme

transformation to the  $\overline{MS}$  scheme, even for  $N_f$  near to  $N_{f,\max}$ .

By construction, since  $b'_3 = 0$  in this scheme, the three-loop zero of  $\beta_{\alpha'}$  is equal to the two-loop zero, as expressed in Eq. (4.4), and as was the case with the  $S_2$  and  $S_3$  schemes. At the four-loop level, the IR zero is given by the physical (smallest positive) solution of the cubic equation (4.5) with  $b'_4$  given by Eq. (3.12) with  $k_1 = k_{1p}$  and  $k_2 = k_3 = 0$ . We list values of  $\alpha'_{\text{IR},n\ell} \equiv \alpha'_{\text{IR},n\ell,S_1}$  in this  $S_1$  scheme, up to ( $n = 4$ )-loop level, as calculated in Ref. [3], in Table I, for relevant  $N_f$ , with fermions in the fundamental representation and several values of  $N$ . For comparison we also include the values of  $\alpha'_{\text{IR},n\ell,\overline{MS}}$  for  $n = 3, 4$  in the  $\overline{MS}$  scheme from Ref. [5].

We carried out the analogous calculations for fermions in the adjoint representation of  $SU(N)$  in Ref. [3]. Here,  $N_{f,b1z} = 11/4$  and  $N_{f,b2z} = 17/16$ , so the only physical, integer value of  $N_f \in I$  is  $N_f = 2$ .  $SU(2)$  models with  $N_f = 2$  adjoint fermions have been of recent interest [43]. For both of these cases we found that

$$\alpha'_{\text{IR},3\ell,S_1} > \alpha'_{\text{IR},3\ell,\overline{MS}}, \quad (5.8)$$

and

$$\alpha'_{\text{IR},4\ell,S_1} < \alpha'_{\text{IR},4\ell,\overline{MS}}. \quad (5.9)$$

For both of these representations, our results obey the required behavior in Eq. (3.10), although one observes that even for rather large  $N_f$  values that are reliably expected to lie in the non-Abelian Coulomb phase, there is still a significant difference between  $\alpha'_{\text{IR},n\ell,S_1}$  and  $\alpha'_{\text{IR},n\ell,\overline{MS}}$  for  $n = 3, 4$ . We attribute this difference to the behavior of  $k_{1p}$  as a function of  $N_f \in I$ . As we will show, this difference is greater than the corresponding difference when one uses a scheme transformation such as the  $S_{\text{sh}}$  scheme to be discussed below.

## VI. THE $S_{\text{th}}$ SCHEME TRANSFORMATION

In this section we study the scheme transformation

$$S_{\text{th}}: a = \frac{\tanh(ra')}{r}. \quad (6.1)$$

Since  $\tanh(ra')/r$  is an even function of  $r$ , we take  $r > 0$  with no loss of generality. The transformation  $S_{\text{th}}$  has the advantage that it depends on a parameter  $r$ , which we can vary to study the effect that it has on the location of the IR fixed point. In particular, as  $r \rightarrow 0$ , this transformation smoothly approaches the identity. The inverse of Eq. (6.1) is

$$a' = \frac{1}{2r} \ln\left(\frac{1+ra}{1-ra}\right), \quad (6.2)$$

and the Jacobian is

$$J = \frac{1}{\cosh^2(ra')}. \quad (6.3)$$

In the notation of Eq. (3.1),

$$f(a') = \frac{\tanh(ra')}{ra'}. \quad (6.4)$$

This has the series expansion of the form (3.2), with

$$k_s = 0 \quad \text{for odd } s, \quad (6.5)$$

and, for even  $s$ ,

$$k_2 = -\frac{r^2}{3}, \quad k_4 = \frac{2r^4}{15}, \quad (6.6)$$

$$k_6 = -\frac{17r^6}{315}, \quad k_8 = \frac{62r^8}{2835}, \quad (6.7)$$

and so forth for  $k_s$  with higher  $s$ .

Substituting these expressions for  $k_s$  into the general expressions for the  $b'_\ell$ , we obtain

$$b'_3 = b_3 + \frac{r^2 b_1}{3}, \quad (6.8)$$

$$b'_4 = b_4, \quad (6.9)$$

$$b'_5 = b_5 - \frac{r^2 b_3}{3} + \frac{2r^4 b_1}{45}, \quad (6.10)$$

$$b'_6 = b_6 - \frac{2r^2 b_4}{3} + \frac{r^4 b_2}{15}, \quad (6.11)$$

$$b'_7 = b_7 - r^2 b_5 + \frac{r^4 b_3}{5} + \frac{r^6 b_1}{315}, \quad (6.12)$$

$$b'_8 = b_8 - \frac{4r^2 b_6}{3} + \frac{4r^4 b_4}{9} - \frac{4r^6 b_2}{189}, \quad (6.13)$$

and so forth for the  $b'_\ell$  with  $\ell \geq 9$ .

We apply this  $S_{\text{th}}$  scheme transformation to the  $\beta$  function in the  $\overline{MS}$  scheme. We will only need the  $b'_\ell$  with  $\ell \leq 4$  for this purpose, since (in addition to the scheme-independent  $b_1$  and  $b_2$ ) only  $b_3$  and  $b_4$  have been calculated for the  $\overline{MS}$  scheme. For  $N_f$  in the interval  $I$  where the two-loop  $\beta$  function has an IR zero, we then calculate the resultant IR zeros in  $\beta_{\alpha'}$  at the three- and four-loop order. We have carried out these calculations for  $N = 2, 3, 4$ , with fermions in the fundamental representation and for a range of  $r$  values, namely  $r = 3, 6, 9$ , and  $4\pi \approx 12.56$ . We list the results in Table II. For  $r = 1$ , the IR zeros are almost identical to those in the  $\overline{MS}$  scheme and hence are not listed. The complex entry for  $N = 2$ ,  $N_f = 7$ ,  $r = 4\pi$  is  $\alpha'_{\text{IR},4\ell,r=4\pi} = 1.718 \pm 0.9285i$ . The presence of this complex entry is a manifestation of the fact pointed out in Ref. [3] and discussed further below that this scheme transformation is not acceptable in general.

TABLE II. Values of the IR zeros of  $\beta_\alpha$  in the  $\overline{MS}$  scheme and  $\beta_{\alpha'}$  after applying the  $S_{\text{th}_r}$  scheme transformation to the  $\overline{MS}$  scheme, for an  $SU(N)$  theory with  $N_f$  fermions in the fundamental representation, for  $N = 2, 3, 4$ , calculated to  $n$ -loop order and denoted as  $\alpha_{\text{IR},n\ell,\overline{MS}}$  and  $\alpha'_{\text{IR},n\ell,S_{\text{th}_r}} \equiv \alpha'_{\text{IR},n\ell,r}$ . The  $S_{\text{th}_r}$  entries are for  $r = 3, 6, 9, 4\pi$ . As before, since the two-loop IR zero is scheme-independent, we denote it simply as  $\alpha_{\text{IR},2\ell}$ .

| $N$ | $N_f$ | $\alpha_{\text{IR},2\ell}$ | $\alpha_{\text{IR},3\ell,\overline{MS}}$ | $\alpha'_{\text{IR},3\ell,r=3}$ | $\alpha'_{\text{IR},3\ell,r=6}$ | $\alpha'_{\text{IR},3\ell,r=9}$ | $\alpha'_{\text{IR},3\ell,r=4\pi}$ | $\alpha_{\text{IR},4\ell,\overline{MS}}$ | $\alpha'_{\text{IR},4\ell,r=3}$ | $\alpha'_{\text{IR},4\ell,r=6}$ | $\alpha'_{\text{IR},4\ell,r=9}$ | $\alpha'_{\text{IR},4\ell,r=4\pi}$ |
|-----|-------|----------------------------|--|---------------------------------|---------------------------------|---------------------------------|------------------------------------|--|---------------------------------|---------------------------------|---------------------------------|------------------------------------|
| 2   | 7     | 2.83                       | 1.05                                     | 1.07                            | 1.11                            | 1.21                            | 1.45                               | 1.21                                     | 1.24                            | 1.33                            | 1.63                            | complex                            |
| 2   | 8     | 1.26                       | 0.688                                    | 0.693                           | 0.706                           | 0.731                           | 0.781                              | 0.760                                    | 0.767                           | 0.789                           | 0.832                           | 0.939                              |
| 2   | 9     | 0.595                      | 0.418                                    | 0.419                           | 0.423                           | 0.428                           | 0.439                              | 0.444                                    | 0.446                           | 0.450                           | 0.458                           | 0.472                              |
| 2   | 10    | 0.231                      | 0.196                                    | 0.196                           | 0.197                           | 0.197                           | 0.199                              | 0.200                                    | 0.200                           | 0.201                           | 0.202                           | 0.203                              |
| 3   | 10    | 2.21                       | 0.764                                    | 0.770                           | 0.786                           | 0.816                           | 0.876                              | 0.815                                    | 0.822                           | 0.844                           | 0.885                           | 0.978                              |
| 3   | 11    | 1.23                       | 0.578                                    | 0.581                           | 0.588                           | 0.602                           | 0.627                              | 0.626                                    | 0.630                           | 0.640                           | 0.660                           | 0.700                              |
| 3   | 12    | 0.754                      | 0.435                                    | 0.436                           | 0.439                           | 0.445                           | 0.456                              | 0.470                                    | 0.472                           | 0.477                           | 0.485                           | 0.502                              |
| 3   | 13    | 0.468                      | 0.317                                    | 0.317                           | 0.318                           | 0.321                           | 0.325                              | 0.337                                    | 0.338                           | 0.340                           | 0.343                           | 0.349                              |
| 3   | 14    | 0.278                      | 0.215                                    | 0.215                           | 0.215                           | 0.216                           | 0.217                              | 0.224                                    | 0.224                           | 0.224                           | 0.225                           | 0.227                              |
| 3   | 15    | 0.143                      | 0.123                                    | 0.123                           | 0.123                           | 0.124                           | 0.124                              | 0.126                                    | 0.126                           | 0.126                           | 0.126                           | 0.126                              |
| 3   | 16    | 0.042                      | 0.040                                    | 0.040                           | 0.040                           | 0.040                           | 0.040                              | 0.040                                    | 0.040                           | 0.040                           | 0.040                           | 0.040                              |
| 4   | 13    | 1.85                       | 0.604                                    | 0.606                           | 0.614                           | 0.627                           | 0.653                              | 0.628                                    | 0.631                           | 0.640                           | 0.656                           | 0.688                              |
| 4   | 14    | 1.16                       | 0.489                                    | 0.491                           | 0.495                           | 0.502                           | 0.516                              | 0.521                                    | 0.523                           | 0.528                           | 0.539                           | 0.557                              |
| 4   | 15    | 0.783                      | 0.397                                    | 0.398                           | 0.401                           | 0.405                           | 0.412                              | 0.428                                    | 0.429                           | 0.433                           | 0.439                           | 0.450                              |
| 4   | 16    | 0.546                      | 0.320                                    | 0.321                           | 0.322                           | 0.324                           | 0.328                              | 0.345                                    | 0.346                           | 0.348                           | 0.351                           | 0.357                              |
| 4   | 17    | 0.384                      | 0.254                                    | 0.254                           | 0.255                           | 0.256                           | 0.258                              | 0.271                                    | 0.271                           | 0.272                           | 0.274                           | 0.277                              |
| 4   | 18    | 0.266                      | 0.194                                    | 0.194                           | 0.195                           | 0.195                           | 0.196                              | 0.205                                    | 0.205                           | 0.205                           | 0.206                           | 0.207                              |
| 4   | 19    | 0.175                      | 0.140                                    | 0.140                           | 0.141                           | 0.141                           | 0.141                              | 0.145                                    | 0.145                           | 0.146                           | 0.146                           | 0.146                              |
| 4   | 20    | 0.105                      | 0.091                                    | 0.091                           | 0.091                           | 0.091                           | 0.091                              | 0.092                                    | 0.092                           | 0.092                           | 0.092                           | 0.093                              |
| 4   | 21    | 0.047                      | 0.044                                    | 0.044                           | 0.044                           | 0.044                           | 0.044                              | 0.044                                    | 0.044                           | 0.044                           | 0.044                           | 0.044                              |

As regards the change in the location of the IR zero as a function of the loop order, we first recall that in Ref. [5] we showed that for a given  $N$  and  $N_f$  (with  $N_f \in I$ , so the two-loop  $\beta$  function has an IR zero), as one goes from two-loop to three-loop order, the location of this zero decreases and then as one goes from three-loop to four-loop order, it increases by a smaller amount, so that the four-loop value is still smaller than the (scheme-independent) 2-loop value. Aside from the pathological behavior that occurs for smaller  $N_f$  values where  $\alpha_{\text{IR},2\ell}$  gets sufficiently large (e.g., for  $N = 2$ ,  $N_f = 7$ , where  $\alpha_{\text{IR},2\ell} = 2.83$  and  $\alpha'_{\text{IR},4\ell,r=4\pi}$  is complex), we observe behavior similar to that which we found in our previous higher-loop calculations for fermions in the fundamental representation in the  $\overline{MS}$  scheme. First, as is evident from Table II, for a given  $N$ ,  $N_f$ , and  $r$ ,

$$\alpha'_{\text{IR},3\ell,S_{\text{th}_r}} < \alpha'_{\text{IR},4\ell,S_{\text{th}_r}} < \alpha_{\text{IR},2\ell} \quad \text{for } R = \text{fund.} \quad (6.14)$$

These shifts as a function of loop order are larger for smaller  $N_f$  and get smaller as  $N_f$  approaches  $N_{f,\text{max}}$ . Second, we observe that for a given  $N$ ,  $N_f$ , and  $r$ ,

$$\alpha'_{\text{IR},n\ell,S_{\text{th}_r}} > \alpha_{\text{IR},n\ell,\overline{MS}}, \quad \text{for } n = 3, 4, \quad R = \text{fund.} \quad (6.15)$$

For a given  $N$  and  $r$ , the values  $\alpha'_{\text{IR},n\ell,S_{\text{th}_r}}$  approach the corresponding  $\alpha_{\text{IR},n\ell,\overline{MS}}$  as  $N_f \nearrow N_{f,\text{max}}$ . Third, for a given  $N$ ,  $N_f$ , and loop order  $n = 3$  or  $n = 4$ ,

$$\alpha'_{\text{IR},n\ell,S_{\text{th}_r}} \text{ is an increasing function of } r. \quad (6.16)$$

For  $N_f$  values close to  $N_{f,\text{max}}$  for a given  $N$ , these differences in values are sufficiently small so that the entries may coincide to the given number of significant figures.

The scheme transformation  $S_{\text{th}_r}$  with  $r = 4\pi$  can be written equivalently as

$$\alpha = \tanh(\alpha'). \quad (6.17)$$

As we pointed out in Ref. [3], the  $S_{\text{th}_r}$  scheme transformation with this value of  $r$  is not acceptable, because it violates conditions  $C_1$ ,  $C_2$ , and  $C_4$ . In particular, as is evident from the inverse of this transformation, viz.,

$$\alpha' = \frac{1}{2} \ln\left(\frac{1 + \alpha}{1 - \alpha}\right), \quad (6.18)$$

the exact inverse transformation maps  $\alpha > 1$  to a complex and hence unphysical, value of  $\alpha'$ . At an IR fixed point, it can easily happen that  $\alpha_{\text{IR},2\ell} > 1$ , in which case this ST yields a complex, unphysical  $\alpha'$ . For example (see Table III in Ref. [5]) for  $G = SU(2)$  with  $N_f = 8$  fermions in the fundamental representation,  $\alpha_{\text{IR},2\ell} = 1.26$  and for  $SU(3)$  with  $N_f = 11$ ,  $\alpha_{\text{IR},2\ell} = 1.23$ . More generally, as is evident from Eq. (6.2), the inverse of the scheme transformation  $S_{\text{th}_r}$  with a given value of  $r$  will map a value  $\alpha > 1$  to a complex, unphysical value of  $\alpha'$  if  $r\alpha/(4\pi) > 1$ . As with the complex entries in Table II, this is another manifestation of the pathology in this scheme transformation at an IR

fixed point. In order for this  $S_{\text{th}}$  scheme transformation to satisfy conditions  $C_1$ ,  $C_2$ , and  $C_4$ , it is necessary that for the values of  $\alpha$  of interest,

$$r < \frac{4\pi}{\alpha} = \frac{1}{a}. \quad (6.19)$$

## VII. THE $S_{\text{sh}}$ SCHEME TRANSFORMATION

In this section we study the scheme transformation

$$S_{\text{sh},r}: a = \frac{\sinh(ra')}{r}. \quad (7.1)$$

Since  $\sinh(ra')/r$  is an even function of  $r$ , we take  $r > 0$  with no loss of generality. This has the inverse

$$a' = \frac{1}{r} \ln \left[ ra + \sqrt{1 + (ra)^2} \right], \quad (7.2)$$

and the Jacobian

$$J = \cosh(ra'). \quad (7.3)$$

In the notation of Eq. (3.1),

$$f(a') = \frac{\sinh(ra')}{ra'}. \quad (7.4)$$

This has a series expansion of the form (3.2) with  $k_s = 0$  for odd  $s$ , as in (6.5), and for even  $s$ ,

$$k_2 = \frac{r^2}{6}, \quad k_4 = \frac{r^4}{120}, \quad (7.5)$$

$$k_6 = \frac{r^6}{5040}, \quad k_8 = \frac{r^8}{362880}, \quad (7.6)$$

and so forth for higher  $s$ .

Substituting these expressions for  $k_s$  into the general expressions for the  $b'_\ell$ , we obtain

$$b'_3 = b_3 - \frac{r^2 b_1}{6}, \quad (7.7)$$

$$b'_4 = b_4, \quad (7.8)$$

$$b'_5 = b_5 + \frac{r^2 b_3}{6} + \frac{31r^4 b_1}{360}, \quad (7.9)$$

$$b'_6 = b_6 + \frac{r^2 b_4}{3} + \frac{r^4 b_2}{15}, \quad (7.10)$$

$$b'_7 = b_7 + \frac{r^2 b_5}{2} + \frac{3r^4 b_3}{40} - \frac{173r^6 b_1}{5040}, \quad (7.11)$$

$$b'_8 = b_8 + \frac{2r^2 b_6}{3} + \frac{r^4 b_4}{9} - \frac{4r^6 b_2}{189}, \quad (7.12)$$

and so forth for the  $b'_\ell$  with  $\ell \geq 9$ .

We apply this  $S_{\text{sh}}$  scheme transformation to the  $\beta$  function in the  $\overline{MS}$  scheme. For the same reason as was given above, we will only need the  $b'_\ell$  with  $\ell \leq 4$  for this purpose. For  $N_f$  in the interval  $I$  where the two-loop  $\beta$  function has an IR zero, we then calculate the resultant IR zeros in  $\beta_{\alpha'}$  at the three- and four-loop order. We have carried out these calculations for  $N = 2, 3, 4$ , with fermions in the fundamental representation and for a range of  $r$  values, namely  $r = 3, 6, 9$ , and  $4\pi$ . We list the results in Table III. We denote the IR zero of  $\beta_{\alpha'}$  at the  $n$ -loop level as  $\alpha'_{\text{IR},n\ell} \equiv \alpha'_{\text{IR},n\ell,S_{\text{sh}}}$ , and in the table we further shorten this to  $\alpha'_{\text{IR},n\ell,r}$ . As with the  $S_{\text{th}}$  scheme transformation, and for the same reason, for  $r = 1$ , the IR zeros are almost identical to those in the  $\overline{MS}$  scheme and hence are not listed.

We observe the following general properties in our calculations of  $\alpha'_{\text{IR},n\ell,S_{\text{sh}}}$ . First, as is evident from Table III, for a given  $N$ ,  $N_f$ , and  $r$ ,

$$\alpha'_{\text{IR},3\ell,S_{\text{sh}}} < \alpha'_{\text{IR},4\ell,S_{\text{sh}}} < \alpha_{\text{IR},2\ell} \quad \text{for } R = \text{fund}. \quad (7.13)$$

As with our calculations with other scheme transformations, these shifts as a function of loop order are larger for smaller  $N_f$  and get smaller as  $N_f$  approaches  $N_{f,\text{max}}$ . Second, for a given  $N$ ,  $N_f$ , and  $r$ ,

$$\alpha'_{\text{IR},n\ell,S_{\text{sh}}} < \alpha_{\text{IR},n\ell,\overline{MS}}, \quad \text{for } n = 3, 4, \quad R = \text{fund}. \quad (7.14)$$

For a given  $N$  and  $r$ , the values  $\alpha'_{\text{IR},n\ell,S_{\text{sh}}}$  approach the corresponding  $\alpha_{\text{IR},n\ell,\overline{MS}}$  as  $N_f \nearrow N_{f,\text{max}}$ . Third, for a given  $N$ ,  $N_f$ , and loop order  $n = 3$  or  $n = 4$ ,

$$\alpha'_{\text{IR},n\ell,S_{\text{sh}}} \text{ is a decreasing function of } r. \quad (7.15)$$

Note that the inequalities (7.14) and (7.15) are opposite to (6.15) and (6.16) for the  $S_{\text{th}}$  scheme transformation. As was the case with the other schemes, for  $N_f$  values close to  $N_{f,\text{max}}$  for a given  $N$ , these properties are sufficiently small so that the entries may coincide to the given number of significant figures.

In contrast with the  $S_{\text{th}}$  scheme transformation, the  $S_{\text{sh}}$  transformation is acceptable for  $r$  values up to the largest that we consider, viz.,  $r = 4\pi$ , where it takes the form

$$\alpha = \sinh(\alpha'). \quad (7.16)$$

This is understandable since the inverse transformation, (7.2), is not singular, whereas the inverse of the  $S_{\text{th}}$  transformation, (7.2), is singular for  $\alpha \rightarrow 1$  for this value of  $r$ . As with the other scheme transformations, the three- and four-loop values of the IR zero in the  $S_{\text{sh}}$  scheme approach the corresponding values in the  $\overline{MS}$  as  $N_f \rightarrow N_{f,\text{max}}$ , in accord with Eq. (3.10).

Some comparative remarks are in order concerning the  $S_1$  and  $S_{\text{sh}}$  scheme transformations. We find that the  $S_{\text{sh}}$  scheme transformation with moderate  $r$  leads to smaller

TABLE III. Values of the IR zeros of  $\beta_\alpha$  in the  $\overline{MS}$  scheme and  $\beta_{\alpha'}$  after applying the  $S_{sh_r}$  scheme transformation to the  $\overline{MS}$  scheme, for an  $SU(N)$  theory with  $N_f$  fermions in the fundamental representation, for  $N = 2, 3, 4$ , calculated to  $n$ -loop order and denoted as  $\alpha_{IR,n\ell,\overline{MS}}$  and  $\alpha'_{IR,n\ell,S_{sh_r}} \equiv \alpha'_{IR,n\ell,r}$ . The  $S_{sh_r}$  entries are for  $r = 3, 6, 9, 4\pi$ . As before, since the two-loop IR zero is scheme-independent, we denote it simply as  $\alpha_{IR,2\ell}$ .

| $N$ | $N_f$ | $\alpha_{IR,2\ell}$ | $\alpha_{IR,3\ell,\overline{MS}}$ | $\alpha'_{IR,3\ell,r=3}$ | $\alpha'_{IR,3\ell,r=6}$ | $\alpha'_{IR,3\ell,r=9}$ | $\alpha'_{IR,3\ell,r=4\pi}$ | $\alpha_{IR,4\ell,\overline{MS}}$ | $\alpha'_{IR,4\ell,r=3}$ | $\alpha'_{IR,4\ell,r=6}$ | $\alpha'_{IR,4\ell,r=9}$ | $\alpha'_{IR,4\ell,r=4\pi}$ |
|-----|-------|---------------------|-----------------------------------|--------------------------|--------------------------|--------------------------|-----------------------------|-----------------------------------|--------------------------|--------------------------|--------------------------|-----------------------------|
| 2   | 7     | 2.83                | 1.05                              | 1.05                     | 1.03                     | 0.998                    | 0.953                       | 1.21                              | 1.20                     | 1.16                     | 1.11                     | 1.04                        |
| 2   | 8     | 1.26                | 0.688                             | 0.686                    | 0.680                    | 0.670                    | 0.654                       | 0.760                             | 0.757                    | 0.747                    | 0.732                    | 0.7085                      |
| 2   | 9     | 0.595               | 0.418                             | 0.418                    | 0.416                    | 0.413                    | 0.409                       | 0.444                             | 0.443                    | 0.441                    | 0.438                    | 0.432                       |
| 2   | 10    | 0.231               | 0.196                             | 0.196                    | 0.196                    | 0.196                    | 0.195                       | 0.200                             | 0.200                    | 0.200                    | 0.200                    | 0.199                       |
| 3   | 10    | 2.21                | 0.764                             | 0.762                    | 0.754                    | 0.742                    | 0.723                       | 0.815                             | 0.812                    | 0.802                    | 0.786                    | 0.762                       |
| 3   | 11    | 1.23                | 0.578                             | 0.577                    | 0.574                    | 0.568                    | 0.559                       | 0.626                             | 0.6245                   | 0.6195                   | 0.611                    | 0.599                       |
| 3   | 12    | 0.754               | 0.435                             | 0.434                    | 0.433                    | 0.430                    | 0.426                       | 0.470                             | 0.470                    | 0.467                    | 0.464                    | 0.457                       |
| 3   | 13    | 0.468               | 0.317                             | 0.316                    | 0.316                    | 0.315                    | 0.313                       | 0.337                             | 0.337                    | 0.336                    | 0.335                    | 0.332                       |
| 3   | 14    | 0.278               | 0.215                             | 0.214                    | 0.214                    | 0.214                    | 0.213                       | 0.224                             | 0.2235                   | 0.223                    | 0.223                    | 0.222                       |
| 3   | 15    | 0.143               | 0.123                             | 0.123                    | 0.123                    | 0.123                    | 0.123                       | 0.126                             | 0.126                    | 0.126                    | 0.126                    | 0.125                       |
| 3   | 16    | 0.042               | 0.040                             | 0.040                    | 0.040                    | 0.040                    | 0.040                       | 0.040                             | 0.040                    | 0.040                    | 0.040                    | 0.040                       |
| 4   | 13    | 1.85                | 0.604                             | 0.602                    | 0.599                    | 0.593                    | 0.583                       | 0.628                             | 0.626                    | 0.622                    | 0.615                    | 0.603                       |
| 4   | 14    | 1.16                | 0.489                             | 0.488                    | 0.486                    | 0.483                    | 0.477                       | 0.521                             | 0.520                    | 0.517                    | 0.513                    | 0.505                       |
| 4   | 15    | 0.783               | 0.397                             | 0.397                    | 0.396                    | 0.394                    | 0.390                       | 0.428                             | 0.428                    | 0.426                    | 0.423                    | 0.419                       |
| 4   | 16    | 0.546               | 0.320                             | 0.320                    | 0.319                    | 0.318                    | 0.316                       | 0.345                             | 0.345                    | 0.344                    | 0.343                    | 0.340                       |
| 4   | 17    | 0.384               | 0.254                             | 0.253                    | 0.253                    | 0.253                    | 0.252                       | 0.271                             | 0.271                    | 0.271                    | 0.270                    | 0.268                       |
| 4   | 18    | 0.266               | 0.194                             | 0.194                    | 0.194                    | 0.194                    | 0.193                       | 0.205                             | 0.205                    | 0.204                    | 0.204                    | 0.2035                      |
| 4   | 19    | 0.175               | 0.140                             | 0.140                    | 0.140                    | 0.140                    | 0.140                       | 0.145                             | 0.145                    | 0.145                    | 0.145                    | 0.145                       |
| 4   | 20    | 0.105               | 0.091                             | 0.091                    | 0.091                    | 0.091                    | 0.091                       | 0.092                             | 0.092                    | 0.092                    | 0.092                    | 0.092                       |
| 4   | 21    | 0.047               | 0.044                             | 0.044                    | 0.044                    | 0.044                    | 0.044                       | 0.044                             | 0.044                    | 0.044                    | 0.044                    | 0.044                       |

shifts in the location of the IR zero than was the case with the  $S_1$  scheme transformation, when both are applied to the  $\beta$  function in the  $\overline{MS}$  scheme. We have explained the origin of this as resulting from a particular feature of the parameter  $k_{1p}$  that enters in the  $S_1$  scheme transformation. In general, we find that even for smaller  $N_f$  values (lying above  $N_{f,b2z}$ ) the  $S_{sh_r}$  transformation with moderate  $r$  produces rather small shifts in the location of the IR zero. For example (cf., Table III), for  $SU(3)$  with  $N_f = 10$ , we obtain the following fractional shifts in this IR zero at the three-loop and four-loop level:

$$\frac{\alpha'_{IR,3\ell,S_{sh_r},r=4\pi} - \alpha_{IR,3\ell,\overline{MS}}}{\alpha_{IR,3\ell,\overline{MS}}} = -0.054$$

$$\frac{\alpha'_{IR,4\ell,S_{sh_r},r=4\pi} - \alpha_{IR,4\ell,\overline{MS}}}{\alpha_{IR,4\ell,\overline{MS}}} = -0.065$$

for  $SU(3)$ ,  $N_f = 10$ ,  $r = 4\pi$ . (7.17)

One would thus tend to prefer the  $S_{sh_r}$  scheme transformation, since it minimizes scheme dependence at higher-loop order. However, the  $S_1$  transformation provides an example of how there may still be significant dependence when one uses certain scheme transformations. We will show another example of this in the next section, using an illustrative exact  $\beta$  function, for which a slight change in  $r$  in the  $S_{sh_r}$

transformation can have a significant effect on the nature of an IR zero at the three-loop order.

## VIII. STUDY WITH AN ILLUSTRATIVE EXACT $\beta$ FUNCTION

It is instructive to study series expansions of an illustrative hypothetical exact  $\beta$  function in order to ascertain the accuracy and reliability of finite-order analyses and the effects of scheme transformations. Here we shall take one such function, which has an exactly known infrared zero that is reached from the origin. It should be emphasized at the outset that, although the function that we use in Eq. (8.4) with (8.6) below is designed to emulate some properties of the  $\beta$  function of an asymptotically free non-Abelian gauge theory with fermions, we do not mean to imply that it is fully realistic. Instead, we use it in the spirit of a reasonable test function which embodies some relevant features and can serve as a theoretical laboratory in which to investigate how well analyses of truncated series expansions probe the IR zero and how this is affected by scheme transformations.

Because we are interested in the evolution of an asymptotically free theory from the neighborhood of the UV fixed point at  $\alpha = 0$  to an IR fixed point, we require that this illustrative  $\beta$  function have the property that, as  $\alpha$  increases from zero, it has a zero at a finite value of  $\alpha$ , which we denote as  $\alpha_{IR}$ . We also require that it be bounded in the interval

$$0 \leq \alpha \leq \alpha_{\text{IR}}. \quad (8.1)$$

It is convenient to define a scaled quantity

$$\tilde{\alpha} \equiv \frac{\alpha}{\alpha_{\text{IR}}}. \quad (8.2)$$

Since we assume that the evolution of the theory from the UV to the IR starts from a small value in the UV, we only need to consider the behavior of  $\beta$  in this interval (8.1). From Eq. (1.2), the  $\beta$  function has the form, for small  $\alpha$  in the deep UV,

$$\begin{aligned} \beta_\alpha &= -2\bar{b}_1\alpha^2 \left[ 1 + \frac{\bar{b}_2}{\bar{b}_1}\alpha + O(\alpha^2) \right] \\ &= -2\bar{b}_1\alpha^2 \left[ 1 - \frac{\alpha}{\alpha_{\text{IR},2\ell}} + O(\alpha^2) \right]. \end{aligned} \quad (8.3)$$

In general, we can write

$$\beta_\alpha = -2\bar{b}_1\alpha^2 h(\alpha), \quad (8.4)$$

where the function  $h(\alpha)$  satisfies

$$h(0) = 1. \quad (8.5)$$

*A priori*, one could consider functions  $h(\alpha)$  with either a finite or an infinite series expansion. We shall consider an illustrative example of the latter case, namely

$$h(\alpha) = \frac{\sin(\pi\sqrt{\tilde{\alpha}})}{(\pi\sqrt{\tilde{\alpha}})}. \quad (8.6)$$

Here we use  $\sqrt{\tilde{\alpha}}$  because  $\sin(x)/x$  has only even powers in its Taylor series expansion

$$\frac{\sin x}{x} = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n}}{(2n+1)!}, \quad (8.7)$$

but we want a  $\beta$  function with odd, as well as even, powers of  $\alpha$ , to emulate a typical  $\beta$  function encountered in a non-Abelian gauge theory. (One could equally well use a similar trigonometric function with this property (and the property (8.5)), such as  $h(\alpha) = \cos[(\pi/2)\sqrt{\tilde{\alpha}}]$ ). As noted above, the feature that (8.6) and this cosine function have an infinite number of zeros beyond the one at  $\tilde{\alpha} = 1$ , i.e.,  $\alpha = \alpha_{\text{IR}}$ , will not be of direct concern to us, since we are only interested in their behavior in the interval (8.1). Although the illustrative  $\beta$  function in Eq. (8.4) with (8.6) has no explicit  $N_f$ -dependence, one may regard it as implicitly incorporating this through the value of  $\alpha_{\text{IR}}$ .

Substituting (8.7) into (8.4), we have, for this illustrative  $\beta$  function,

$$\beta_\alpha = -2\bar{b}_1\alpha^2 \sum_{\ell=1}^{\infty} \frac{(-\pi^2\alpha/\alpha_{\text{IR}})^{\ell-1}}{(2\ell-1)!}. \quad (8.8)$$

Hence, in the notation of Eq. (1.2),

$$\frac{\bar{b}_\ell}{\bar{b}_1} = \frac{(-\pi^2/\alpha_{\text{IR}})^{\ell-1}}{(2\ell-1)!}, \quad (8.9)$$

or equivalently,

$$\frac{b_\ell}{b_1} = \frac{(-4\pi^3/\alpha_{\text{IR}})^{\ell-1}}{(2\ell-1)!}. \quad (8.10)$$

Before performing a scheme transformation, we first analyze finite-order truncations of this  $\beta$  function to see how closely the resulting determination of the IR zero compares with the exact value,  $\alpha_{\text{IR}}$ . Obviously, no claim is made that this  $\beta$  function actually arose from a loop calculation, but it will be useful to employ the terminology of loops to refer to the expansion order. To four-loop order,  $\ell = 4$ , Eq. (1.2) reads

$$\beta_\alpha = -2\bar{b}_1\alpha^2 \left[ 1 + \frac{\bar{b}_2}{\bar{b}_1}\alpha + \frac{\bar{b}_3}{\bar{b}_1}\alpha^2 + \frac{\bar{b}_4}{\bar{b}_1}\alpha^3 + O(\alpha^4) \right]. \quad (8.11)$$

Explicitly,

$$\beta_\alpha = -2\bar{b}_1\alpha^2 \left[ 1 - \frac{\pi^2}{3!}\tilde{\alpha} + \frac{\pi^4}{5!}\tilde{\alpha}^2 - \frac{\pi^6}{7!}\tilde{\alpha}^3 + O(\tilde{\alpha}^4) \right]. \quad (8.12)$$

For our further discussion, we shall define a compact notation consistent with Eq. (8.2), namely

$$\tilde{\alpha}_{\text{IR},n\ell} \equiv \frac{\alpha_{\text{IR},n\ell}}{\alpha_{\text{IR}}}. \quad (8.13)$$

At the two-loop order, the  $\beta$  function given in Eqs. (8.11) and (8.12) has an IR zero at  $\alpha_{\text{IR},2\ell} = -\bar{b}_1/\bar{b}_2 = (6/\pi^2)\alpha_{\text{IR}} = 0.60793\alpha_{\text{IR}}$ , i.e.,

$$\tilde{\alpha}_{\text{IR},2\ell} = 0.60793, \quad (8.14)$$

to the indicated numerical accuracy. Evidently, this two-loop estimate of the IR zero differs substantially from the exact value of the IR zero, being approximately 40% smaller than this value. Interestingly, at the three-loop level, although  $\beta_\alpha$  has two zeros at nonzero values of  $\tilde{\alpha}$ , neither of them is a physical IR zero; instead, they form the complex-conjugate pair

$$\tilde{\alpha}_{\text{IR},3\ell,\pm} = \frac{2(5 \pm \sqrt{5}i)}{\pi^2} = 1.0132 \pm 0.4531i. \quad (8.15)$$

This is an important result, since it illustrates the basic fact from calculus that a polynomial obtained as a truncation of a series expansion for a given function does not necessarily accurately reproduce the zeros of that function. In the present case, the real part of the complex pair of zeros is rather close to 1, but the imaginary part is not small relative to this real part, so that in the complex plane, the distance of each of these roots from 1, i.e., the distance of the roots in  $\alpha$  from  $\alpha_{\text{IR}}$ , is substantial. At four-loop order, the  $\beta_\alpha$  function has three nonzero roots in  $\tilde{\alpha}$ , namely a physical IR zero close to the exact value,

$$\tilde{\alpha}_{\text{IR},4\ell} = 0.9603, \quad (8.16)$$

about 4% smaller than the exact value, together with a complex conjugate pair at  $\tilde{\alpha} = 1.6476 \pm 1.6566i$ .

We have continued this analysis up to ( $n = 8$ )-loop order. At five-loop level, the equation  $\beta_\alpha = 0$  has a real root very close to the exact value,

$$\tilde{\alpha}_{\text{IR},5\ell} = 1.0045, \quad (8.17)$$

together with another real root at  $\tilde{\alpha} = 2.4958$  and a complex pair,  $\tilde{\alpha} = 1.8974 \pm 3.4138i$ . At the six-loop level, the equation  $\beta_\alpha = 0$  has five nonzero solutions for  $\tilde{\alpha}$ , namely

$$\tilde{\alpha}_{\text{IR},6\ell} = 0.99972, \quad (8.18)$$

and two pairs of complex-conjugate roots. At the seven-loop level, the equation  $\beta_\alpha = 0$  has the root

$$\tilde{\alpha}_{\text{IR},7\ell} = 1.00001346, \quad (8.19)$$

together with two pairs of complex-conjugate roots and a larger positive real root at  $\tilde{\alpha} = 3.621288$ . Finally, at the eight-loop level, the equation  $\beta_\alpha = 0$  yields

$$\tilde{\alpha}_{\text{IR},8\ell} = 0.999999507, \quad (8.20)$$

together with two pairs of complex-conjugate roots and two larger real roots. These values of the physical IR zero for  $4 \leq \ell \leq 8$  yield the following fractional differences with respect to the exact value:

$$\tilde{\alpha}_{\text{IR},4\ell} - 1 \equiv \frac{\alpha_{\text{IR},4\ell} - \alpha_{\text{IR}}}{\alpha_{\text{IR}}} = -3.97 \times 10^{-2}, \quad (8.21)$$

$$\frac{\alpha_{\text{IR},5\ell} - \alpha_{\text{IR}}}{\alpha_{\text{IR}}} = 4.52 \times 10^{-3}, \quad (8.22)$$

$$\frac{\alpha_{\text{IR},6\ell} - \alpha_{\text{IR}}}{\alpha_{\text{IR}}} = -2.83 \times 10^{-4}, \quad (8.23)$$

$$\frac{\alpha_{\text{IR},7\ell} - \alpha_{\text{IR}}}{\alpha_{\text{IR}}} = 1.35 \times 10^{-5}, \quad (8.24)$$

and

$$\frac{\alpha_{\text{IR},8\ell} - \alpha_{\text{IR}}}{\alpha_{\text{IR}}} = -0.493 \times 10^{-6}. \quad (8.25)$$

Thus, once one gets beyond the three-loop order, these values converge monotonically toward the exact value of  $\alpha_{\text{IR}}$ .

We next perform a scheme transformation on  $\beta_\alpha$  and study the shift in the values of the IR zero of  $\beta_{\alpha'}$ , calculated to the various orders considered here. We denote these as  $\alpha'_{\text{IR},n\ell}$  and the ratios with respect to  $\alpha_{\text{IR}}$  as  $\tilde{\alpha}'_{\text{IR},n\ell}$ . For definiteness, we use the  $S_{\text{sh}_r}$  transformation given in Eq. (7.1), i.e.,  $\alpha = (4\pi/r) \sinh(r\alpha'/(4\pi))$ , with variable  $r$ . As noted before, without loss of generality, we may take  $r > 0$ . Clearly, as  $r \rightarrow 0^+$ , the  $S_{\text{sh}_r}$  scheme transformation approaches the identity map, so, by continuity, in this limit, the resulting values of the IR zero calculated at the  $\ell$ -loop

level approach those obtained above. However, as we will show next, the values that one gets for larger  $r$  depend sensitively on this parameter. Of course, at the two-loop level, since  $b'_\ell = b_\ell$  for  $\ell = 1, 2$ , we get the zero at the same place, but now in the  $\alpha'$  variable, namely,

$$\tilde{\alpha}'_{\text{IR},2\ell,S_{\text{sh}_r}} = 0.60793. \quad (8.26)$$

At the three-loop level, the condition  $\beta_{\alpha'} = 0$  yields (aside from the double root at  $\alpha' = 0$  corresponding to the UV fixed point), the quadratic equation

$$1 - \frac{\pi^2}{6} \tilde{\alpha}' + \left( \frac{\pi^4}{120} - \frac{r^2}{96\pi^2} \right) (\tilde{\alpha}')^2 = 0. \quad (8.27)$$

This equation obviously has a singular behavior at the value of  $r$  that causes the coefficient of the  $(\tilde{\alpha}')^2$  term to vanish, namely  $r = 2\pi^3/\sqrt{5} = 27.73 \dots$  We assume that  $r$  does not take on this value. The equation then has the two formal solutions,

$$\tilde{\alpha}'_{\text{IR},3\ell} = \frac{20\pi^3 \pm \sqrt{150r^2 - 20\pi^6}}{4\pi} \frac{1}{2(4\pi^6 - 5r^2)}. \quad (8.28)$$

We showed above that in the analysis of  $\beta_\alpha$  at this three-loop level, there are no real roots. Here, in contrast, for sufficiently large  $r$ , these roots become real. This demonstrates how a scheme transformation can qualitatively, as well as quantitatively, change the analysis of the IR zero of a  $\beta$  function. In the present case, the roots are real if the discriminant is nonnegative, i.e., if

$$r \geq \left( \frac{2}{15} \right)^{1/2} \pi^3 = 11.322. \quad (8.29)$$

In order to get real roots at the three-loop level, we restrict to  $r$  values that satisfy this inequality. For example, let us take  $r = 4\pi$ . Then from Eq. (8.28) we obtain an IR zero at

$$\tilde{\alpha}'_{\text{IR},3\ell,S_{\text{sh}_r}} = 1.000400 \quad \text{for } r = 4\pi, \quad (8.30)$$

together with another real root  $\tilde{\alpha}' = 1.54959$ . Although the three-loop value in Eq. (8.28) is very close to the exact value 1, i.e.,  $\alpha'_{\text{IR},3\ell,S_{\text{sh}_r}}$  is very close to  $\alpha_{\text{IR}}$ , this is fortuitous.

For example, if one increases  $r$  from  $4\pi = 12.566$  slightly to  $r = 15$ , the value in Eq. (8.30) shifts to  $\tilde{\alpha}'_{\text{IR},3\ell,S_{\text{sh}_r}} = 1.19414$ . If, on the other hand, one decreases  $r$  to ostensibly reasonable values below the lower bound (8.29), then one would revert back to the situation encountered in the analysis of  $\beta_\alpha$ , namely there would not be any physical IR zero at this three-loop level.

At the four-loop level, if one continues to use the value  $r = 4\pi$ , the condition  $\beta_{\alpha'} = 0$  yields one real root, which is the IR zero,

$$\tilde{\alpha}'_{\text{IR},4\ell,S_{\text{sh}_r}} = 0.79922 \quad \text{for } r = 4\pi, \quad (8.33)$$

together with a pair of complex-conjugate roots. One can carry this analysis to higher-loop level. For example, at five-loop level, with  $r = 4\pi$ , the condition  $\beta_{\alpha'} = 0$  yields



not real solutions for an IR zero, but instead a quartic equation with two pairs of complex-conjugate roots.

In closing this section, we again emphasize that we have carried out this analysis in the spirit of using a test function with reasonable behavior in the relevant interval (8.1) to study how well analyses of a finite series expansion probe its IR zero, and the effect of a scheme transformation on these. There is obviously no implication that other properties of the particular test function (8.4) with (8.6) (such as the infinitely many zeros at  $\sqrt{\alpha} = s$  with  $s \geq 2$ ) are relevant to the true  $\beta$  function of a non-Abelian gauge theory.

### IX. ANOMALOUS DIMENSION OF FERMION BILINEAR

The anomalous dimension  $\gamma_m$  describes the scaling of a fermion bilinear and the running of a dynamically generated fermion mass in the phase with spontaneous chiral symmetry breaking. It plays an important role in technicolor theories, via the renormalization group factor  $\eta = \exp[\int dt \gamma_m(\alpha(t))]$  that can enhance dynamically generated Standard-Model fermion masses. In the non-Abelian Coulomb phase (which is a conformal phase), the IR zero of  $\beta$  is exact, although a calculation of it to a finite-order in perturbation theory is only approximate, and  $\gamma_m$  evaluated at this IR fixed point is exact. In the phase with  $S_\chi$ SB, where an IR fixed point, if it exists, is only approximate,  $\gamma_m$  is an effective quantity describing the running of a dynamically generated fermion mass for the evolution of the theory near this approximate IRFP. In Ref. [5] we evaluated  $\gamma_m$  to three- and four-loop order at the IR zero of  $\beta$  calculated to the same order and showed that these higher-loop results were somewhat smaller than the two-loop evaluation. In both the conformal and non-conformal phases it is important to assess the scheme-dependence of  $\gamma_m$  when calculated to finite order. At an exact zero of  $\beta$ , the anomalous dimension  $\gamma_m(\alpha)$  calculated in a given scheme is the same as the anomalous dimension  $\gamma'_m(\alpha')$  calculated in another scheme [9]. Our results in Ref. [3] and here concerning shifts in the location of the IR zero resulting from a scheme transformation show that, *a priori*, a transformation may introduce significant shifts in both this location and in the resultant value of  $\gamma_m$ , especially when the IR fixed point occurs at moderate to strong coupling. For a given gauge group  $G$  and fermion representation  $R$ , the value of  $\alpha_{\text{IR},2\ell}$  gets larger as  $N_f \searrow N_{f,b2z}$ , and hence, understandably, the shift in  $\alpha'_{\text{IR},n\ell}$  when calculated in a different scheme can be significant. The same comment applies to  $\gamma_m$ , although part of this region of  $N_f \gtrsim N_{f,b2z}$  is in the phase with spontaneous chiral symmetry breaking rather than the chirally symmetric phase, so the IR fixed point is only approximate. For a well-behaved scheme transformation such as  $S_{\text{sh},r}$  with moderate  $r$ , as  $N_f$  increases throughout the non-Abelian Coulomb phase, this scheme-dependent shift in a finite-loop-order calculation

of the IR zero and resultant shift in the value of  $\gamma_m$ , calculated to the same finite-loop order, become small.

### X. DISCUSSION AND CONCLUSIONS

In this paper, extending the work in Ref. [3], we have given a detailed analysis of the effects of scheme transformations in the vicinity of an exact or approximate infrared fixed point in an asymptotically free gauge theory with fermions. We have discussed a set of necessary conditions that such transformations must obey and have shown with several examples that, although these can easily be satisfied in the vicinity of an ultraviolet fixed point, they constitute significant restrictions on scheme transformations at an infrared fixed point. This is especially true when this fixed point occurs at a relatively strong coupling.

We have constructed acceptable scheme transformations and have used these to study the scheme-dependence of an infrared fixed point, making comparison with our previous three-loop and four-loop calculations of the location of this point in the  $\overline{MS}$  scheme in Ref. [5]. The  $S_1$  transformation, which renders the three-loop coefficient of the  $\beta_{\alpha'}$  function zero, provides an example of how a scheme transformation can produce significant scheme dependence in an IR zero. The  $S_{\text{sh},r}$  scheme transformation with moderate  $r$  is better behaved than the  $S_1$  transformation and introduces smaller scheme-dependent shifts in the location of the IR zero. This  $S_{\text{sh},r}$  transformation with moderate  $r$  provides a valuable tool to assess scheme dependence. As applied to the  $\beta$  function in the  $\overline{MS}$  scheme, it shows that this dependence is small in the vicinity of both the UV fixed point at  $\alpha = 0$  and an IR fixed point at sufficiently small coupling. It also gives a quantitative measure of the size of the scheme-dependence in the calculation of this fixed point at the three-loop and four-loop order, both at small and at larger couplings.

We have constructed an illustrative exact  $\beta$  function of an asymptotically free theory with an infrared zero and have used it as a theoretical laboratory in which to assess the accuracy with which finite-order truncations of the series expansion of this  $\beta$  function are able to determine the IR zero. Applying the  $S_{\text{sh},r}$  scheme transformation to the series expansion for this illustrative  $\beta$  function, we have also studied the consequences of this for the determination of the IR zero in the  $\alpha'$  variable from a finite-order truncation of the series. For the illustrative  $\beta$  function, we find that this scheme transformation can have a significant effect, especially at low orders in the expansion.

We believe that the results reported here give a deeper insight into scheme transformations of the  $\beta$  function and scheme-dependence of infrared fixed points in non-Abelian gauge theories with fermions. There is clearly more interesting work to be done investigating this question. The knowledge gained will be useful for a better understanding of the UV to IR evolution of these theories, in particular, those with fermion contents that result in quasi-conformal behavior.

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## APPENDIX

In this appendix we first give the expressions that we have calculated for  $b'_\ell$  with  $\ell = 6, 7, 8$ :

$$b'_6 = b_6 + 4k_1b_5 + (4k_1^2 + 2k_2)b_4 + 4k_1k_2b_3 + (2k_1^4 - 6k_1^2k_2 + 4k_1k_3 + 3k_2^2 - 2k_4)b_2 + (-8k_1^5 + 28k_1^3k_2 - 16k_1^2k_3 - 20k_1k_2^2 + 8k_1k_4 + 12k_2k_3 - 4k_5)b_1, \quad (\text{A1})$$

$$b'_7 = b_7 + 5k_1b_6 + (7k_1^2 + 3k_2)b_5 + (2k_1^3 + 7k_1k_2 + k_3)b_4 + (k_1^4 - 2k_1^2k_2 + 4k_1k_3 + 3k_2^2 - k_4)b_3 + (-4k_1^5 + 15k_1^3k_2 - 9k_1^2k_3 - 12k_1k_2^2 + 9k_2k_3 + 5k_1k_4 - 3k_5)b_2 + (16k_1^6 - 68k_1^4k_2 + 40k_1^3k_3 - 21k_1^2k_4 + 73k_1^2k_2^2 - 58k_1k_2k_3 + 10k_1k_5 + 16k_2k_4 - 12k_2^3 + 9k_3^2 - 5k_6)b_1, \quad (\text{A2})$$

and

$$b'_8 = b_8 + 6k_1b_7 + (11k_1^2 + 4k_2)b_6 + (6k_1^3 + 12k_1k_2 + 2k_3)b_5 + (k_1^4 + 4k_1^2k_2 + 6k_1k_3 + 4k_2^2)b_4 + (-2k_1^5 + 8k_1^3k_2 - 4k_1^2k_3 - 6k_1k_2^2 + 8k_2k_3 + 4k_1k_4 - 2k_5)b_3 + (8k_1^6 - 36k_1^4k_2 + 22k_1^3k_3 - 12k_1^2k_4 + 42k_1^2k_2^2 - 36k_1k_2k_3 + 6k_1k_5 + 12k_2k_4 - 8k_2^3 + 7k_3^2 - 4k_6)b_2 + (-32k_1^7 + 160k_1^5k_2 - 96k_1^4k_3 + 52k_1^3k_4 - 230k_1^3k_2^2 - 26k_1^2k_5 + 208k_1^2k_2k_3 + 12k_1k_6 + 84k_1k_2^3 - 42k_1k_3^2 - 76k_1k_2k_4 + 20k_2k_5 + 24k_3k_4 - 52k_2^2k_3 - 6k_7)b_1. \quad (\text{A3})$$

For reference, we list the expressions for  $b_1$  [7],  $b_2$  [8], and, in the  $\overline{MS}$  scheme,  $b_3$  [13], calculated for a vectorial gauge theory with  $N_f$  (massless) fermions transforming according to the representation  $R$  of the gauge group  $G$  [25]:

$$b_1 = \frac{1}{3}(11C_A - 4T_fN_f) \quad (\text{A4})$$

$$b_2 = \frac{1}{3}[34C_A^2 - 4(5C_A + 3C_f)T_fN_f]. \quad (\text{A5})$$

$$b_3 = \frac{2857}{54}C_A^3 + T_fN_f\left[2C_f^2 - \frac{205}{9}C_AC_f - \frac{1415}{27}C_A^2\right] + (T_fN_f)^2\left[\frac{44}{9}C_f + \frac{158}{27}C_A\right]. \quad (\text{A6})$$

In our calculations we have also used the  $\overline{MS}$  result for  $b_4$  [14], but we do not list it here because of its length.

The interval  $I$  in which the two-loop  $\beta$  function has an IR zero is given in Eq. (2.4). The lower end of this interval is defined by the condition that  $b_2$  decreases through zero, which occurs at the value  $N_f = N_{f,b2z}$  given in Eq. (2.3). Numerical values of  $\bar{b}_\ell$  were presented in Ref. [5], e.g., for the fundamental representation in Table I of that reference. As discussed in Ref. [5], for  $N_f = 0$  and sufficiently small,  $b_2$ ,  $b_3$ , and  $b_4$  are all positive, and they decrease with increasing  $N_f$ . The value of  $N_f$  at which  $b_3$  goes through zero and becomes negative, denoted  $N_{f,b3z}$ , is smaller than the value  $N_{f,b2z}$ , so that  $b_3$  is generically negative in the interval  $I$  [cf., Eq. (2.4)] where the two-loop  $\beta$  function has an IR zero. As is evident in Table I, the four-loop

coefficient  $b_4$  can be positive or negative in this interval  $I$ . The upper end of the interval  $I$  occurs at  $N_f = N_{f,b1z} = N_{f,\max}$  [26], where  $b_1 \rightarrow 0^+$ . The values of  $b_2$  and  $b_3$  at  $N_f = N_{f,\max}$  are used implicitly in the text, in particular, in our discussion of the  $S_1$  scheme transformation, so we list them here:

$$b_2 = -C_A(7C_A + 11C_f) \quad \text{at } N_f = N_{f,\max}, \quad (\text{A7})$$

and

$$b_3 = -\frac{C_A}{24}(1127C_A^2 + 616C_AC_f - 132C_f^2) \quad \text{at } N_f = N_{f,\max}. \quad (\text{A8})$$

We denote these as  $(b_2)_{N_{f,\max}}$  and  $(b_3)_{N_{f,\max}}$ , respectively. For the fundamental representation,

$$(b_2)_{N_{f,\max},\text{fund}} = -\left[\frac{(5N)^2 - 11}{2}\right], \quad (\text{A9})$$

and

$$(b_3)_{N_{f,\max},\text{fund}} = -\left[\frac{1402N^4 - 242N^2 - 33}{24N}\right]. \quad (\text{A10})$$

These are both negative for all physically relevant  $N$ . Specifically, with  $N_f$  continued from the nonnegative integers to the nonnegative reals,

$$(b_2)_{N_{f,\max},\text{fund}} < 0 \quad \text{for } N > \frac{\sqrt{11}}{5} = 0.66332, \quad (\text{A11})$$

and

$$(b_3)_{N_f, \text{max, fund.}} < 0$$

$$\text{for } N > \frac{[169642 + 9814\sqrt{1243}]^{1/2}}{1402} = 0.512186. \quad (\text{A12})$$

For the adjoint representation,

$$(b_2)_{N_f, \text{max, adj}} = -18N^2, \quad (\text{A13})$$

and

$$(b_3)_{N_f, \text{max, fund.}} = -\frac{537N^3}{8}, \quad (\text{A14})$$

which are also negative.

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