

**Study of scheme transformations to remove higher-loop terms in the  $\beta$  function of a gauge theory**

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(Received 28 May 2013; published 6 August 2013)

Since three-loop and higher-loop terms in the  $\beta$  function of a gauge theory are scheme-dependent, one can, at least for sufficiently small coupling, carry out a scheme transformation that removes these terms. A basic question concerns the extent to which this can be done at an infrared fixed point of an asymptotically free gauge theory. This is important for quantitative analyses of the scheme dependence of such a fixed point. Here we study a scheme transformation  $S_{R,m}$  with  $m \geq 2$  that is constructed so as to remove the terms in the beta function at loop order  $\ell = 3$  to  $\ell = m + 1$ , inclusive. Starting from an arbitrary initial scheme, we present general expressions for the coefficients of terms of loop order  $\ell$  in the beta function in the transformed scheme from  $\ell = m + 2$  up to  $\ell = 8$ . Extending a previous study of  $S_{R,2}$ , we investigate the range of applicability of the  $S_{R,3}$  scheme transformation in an asymptotically free  $SU(N_c)$  gauge theory with an infrared zero in  $\beta$  depending on the number,  $N_f$ , of fermions in the theory. We show that this  $S_{R,3}$  scheme transformation can only be applied self-consistently in a restricted range of  $N_f$  with a correspondingly small value of infrared fixed-point coupling. We also study the effect of higher-loop terms on the beta function of a  $U(1)$  gauge theory.

DOI: [10.1103/PhysRevD.88.036003](https://doi.org/10.1103/PhysRevD.88.036003)

PACS numbers: 11.10.Hi, 11.15.-q, 11.15.Bt

**I. INTRODUCTION**

The evolution of the coupling  $g(\mu)$  as a function of the reference Euclidean momentum scale,  $\mu$ , from the ultraviolet (UV) to the infrared (IR) in an asymptotically free (AF) gauge theory is of fundamental field-theoretic importance. This evolution of  $g(\mu)$ , or equivalently,  $\alpha(\mu) = g(\mu)^2/(4\pi)$ , is described by the  $\beta$  function of the theory. Terms at loop order  $\ell \geq 3$  in the  $\beta$  function are dependent on the scheme used for regularization and renormalization. Hence, one expects that, at least for sufficiently small coupling, it is possible to carry out a scheme transformation that removes these terms and yields a  $\beta$  function with only one- and two-loop terms [1]. In [2] we constructed what is, to our knowledge, the first explicit scheme transformation that removes terms at loop order  $\ell \geq 3$  from the beta function, at least in the vicinity of the UV fixed point at  $\alpha = 0$ .

An important application of such a scheme transformation is to asymptotically free gauge theories that have an infrared zero in the  $\beta$  function. Depending on how large the value of the coupling is at this IR zero, it is either an exact or approximate fixed point of the renormalization group of the theory. In order to understand the physical implications of this IR zero, it is necessary to assess the effect of scheme dependence on its value. Hence, a crucial question concerning a scheme transformation designed to remove terms at three- and higher-loop order in the beta function, is whether one can use it in the vicinity of an IR zero of this function. Indeed, a scheme transformation that is acceptable for small coupling can produce unphysical effects that render it inapplicable for somewhat larger couplings [2].

Here we study a scheme transformation  $S_{R,m}$  with  $m \geq 2$  that is constructed so as to remove the  $\ell$ -loop terms in the beta function at loop order  $\ell = 3$  to  $\ell = m + 1$ , inclusive. We investigate this to the highest-loop order possible using known coefficients of  $\beta$  for a non-Abelian gauge theory, namely  $\ell = 4$  loop order, corresponding to  $m = 3$ . We focus on an asymptotically free gauge theory with gauge group  $SU(N_c)$  containing  $N_f$  massless fermions in the fundamental representation, although many of our results apply to the case of an arbitrary gauge group  $G$  with  $N_f$  massless fermions in a general representation  $R$  of  $G$  [3]. Starting from an arbitrary initial scheme, we present general expressions for the coefficients of terms of loop order  $\ell$  in the beta function in the transformed scheme from  $\ell = m + 2$  up to  $\ell = 8$ . It was shown in [2] that the  $S_{R,2}$  scheme transformation has a limited range of applicability and cannot be used for a substantial subset of  $N_f$  values where the theory has an IR zero in  $\beta$  because it produces unphysical effects, namely a reversal of the sign of  $\alpha$ . This finding naturally leads to a question: how general is this problem and can one alleviate or circumvent it by using the higher-order scheme transformation  $S_{R,3}$ ?

We address and answer this question here. We will show here that the problem is generically still present with the  $S_{R,3}$  scheme transformation. For example, we will show that for a theory with gauge group  $SU(3)$  and  $N_f = 12$  fermions, one cannot use the  $S_{R,3}$  scheme transformation in the vicinity of the (scheme-independent) IR zero of the two-loop  $\beta$  function because it produces the same type of unphysical results that the  $S_{R,2}$  transformation does. Thus, while it is true that one can remove terms at loop order  $\ell \geq 3$  in a  $\beta$  function for sufficiently small  $\alpha$ , one must take considerable care in attempting such a scheme

transformation at moderate values of  $\alpha$  relevant for a generic infrared fixed point. As part of our work, we also discuss some higher-loop properties of the  $\beta$  function and associated issues of scheme dependence for a U(1) gauge theory.

This paper is organized as follows. In Sec. II we give some additional background and motivations for the current work. The definition and some properties of a general scheme transformation are presented in Sec. III. In Sec. IV we define the scheme transformation  $S_{R,m}$  that, at least for sufficiently small  $\alpha$ , removes terms in the beta function from loop order  $\ell = 3$  to  $\ell = m + 1$ , inclusive. Explicit expressions for the resultant coefficients in the new scheme are presented in Sec. V. In Sec. VI we discuss the range of applicability of the transformation  $S_{R,2}$  at an IR zero of the beta function. In Sec. VII we present our results on the range of applicability of the  $S_{R,3}$  scheme transformation. As discussed in Sec. VIII, further insights concerning the range of applicability of these scheme transformations are gained by studying the limit of an SU( $N_c$ ) gauge theory with  $N_f$  fermions in the fundamental representation in the limit  $N_c \rightarrow \infty$ ,  $N_f \rightarrow \infty$  with the ratio  $N_f/N_c$  fixed. In Sec. IX we discuss some higher-loop properties of the  $\beta$  function for a U(1) gauge theory. Our conclusions are given in Sec. X, and some additional relevant formulas are listed in several appendices.

## II. BACKGROUND

The dependence of  $\alpha(\mu)$  on  $\mu$  is described by the  $\beta$  function [4,5]

$$\beta \equiv \beta_\alpha = \frac{d\alpha}{dt}, \quad (2.1)$$

where  $t = \ln \mu$ . It will be convenient to introduce the quantity  $a(\mu) \equiv \alpha(\mu)/(4\pi) = g(\mu)^2/(16\pi^2)$  (the argument  $\mu$  will often be suppressed in the notation). The  $\beta$  function has the expansion

$$\beta_\alpha = -2\alpha \sum_{\ell=1}^{\infty} b_\ell a^\ell = -2\alpha \sum_{\ell=1}^{\infty} \bar{b}_\ell \alpha^\ell, \quad (2.2)$$

where

$$\bar{b}_\ell = \frac{b_\ell}{(4\pi)^\ell}. \quad (2.3)$$

The  $n$ -loop  $\beta$  function is given by Eq. (2.2) with the upper limit on the  $\ell$  loop summation equal to  $n$  instead of  $\infty$ . The one-loop and two-loop coefficients,  $b_1$  and  $b_2$ , are independent of the scheme used for regularization and renormalization, while  $b_\ell$  with  $\ell \geq 3$  are scheme-dependent [6]. The coefficients  $b_1$  and  $b_2$  were calculated for a non-Abelian Yang-Mills gauge theory in [7] and [8,9]. Dimensional regularization [10] and minimal subtraction [11] are particularly convenient for these loop calculations. Calculations of  $b_3$  and  $b_4$  in the modified minimal

subtraction scheme, denoted  $\overline{\text{MS}}$  [12], were given in [13–15]. We recall that perturbative expansions in quantum field theory, such as Eq. (2.2), are, in general, asymptotic expansions rather than Taylor series expansions with finite radii of convergence. However, a wealth of experience with the use of perturbation theory for calculations of electro-weak cross sections and decay rates and for perturbative calculations in quantum chromodynamics (QCD), has shown that these expansions can give reasonably accurate results and that this accuracy increases when one carries these computations to higher-loop order. Extensive studies have been performed on the scheme dependence and related scale dependence of perturbative QCD calculations [16].

If an asymptotically free gauge theory has sufficiently many massless fermions, the  $\beta$  function can exhibit an IR zero at a certain value, denoted  $\alpha_{\text{IR}}$  [8,17,18]. If  $\alpha_{\text{IR}}$  is sufficiently small, then this is an exact IR fixed point (IRFP) of the renormalization group, and the UV to IR evolution can be computed with reasonable accuracy, since the theory starts with weak coupling in the deep UV and never becomes strongly coupled. As the number of fermions,  $N_f$ , is decreased,  $\alpha_{\text{IR}}$  increases. For a theory with sufficiently few fermions, as  $\mu$  decreases past a scale denoted as  $\Lambda$ ,  $\alpha(\mu)$  becomes large enough to trigger the formation of bilinear fermion condensates that break the global chiral symmetry. In a vectorial gauge theory, these condensates are gauge invariant, while in a chiral gauge theory, if the condensates form, then they generically break the gauge symmetry [19]. Henceforth, for simplicity, we focus on the case of a vectorial gauge theory. Associated with this condensate formation, the fermions involved in the condensates gain dynamical masses of order  $\Lambda$ . In the low-energy effective field theory applicable at scales  $\mu < \Lambda$ , one integrates out these now-massive fermions, and the  $\beta$  function reverts to that of a pure gauge theory, which has no (perturbative) IR zero. Thus, in this case the formal IR zero in  $\beta$  is only approximate. As  $N_f$  decreases through a critical number,  $N_{f,\text{cr}}$ , the theory can be regarded as undergoing a (zero-temperature) phase transition from chirally symmetric to chirally broken infrared behavior. If  $\alpha_{\text{IR}}$  is only slightly greater than the critical value for fermion condensation, then the theory exhibits a slowly running coupling and associated quasiscale invariant behavior [20].

To investigate the properties of a theory with an IR fixed point at moderate coupling, it is necessary to calculate the value of  $\alpha_{\text{IR}}$  to higher-loop order [21]. This was done up to four-loop order for  $\alpha_{\text{IR}}$  and the anomalous dimension,  $\gamma_m$ , of the fermion bilinear for a general gauge group and fermion representation in [22,23]. Further higher-loop results on structural properties of  $\beta$  were calculated in [24–26]. Because the coefficients  $b_\ell$  for  $\ell \geq 3$  are scheme-dependent, it is necessary to assess quantitatively how important the effect of this scheme dependence is on

the location of  $\alpha_{\text{IR}}$ . This task was carried out in [2]. To do this, one constructs a scheme transformation, applies it, calculates the value of  $\alpha'_{\text{IR}}$  in the new scheme, and determines how much  $\alpha'_{\text{IR}}$  differs from  $\alpha_{\text{IR}}$  to a given loop order.

However, one encounters a significant complication in this program of constructing and performing various scheme transformations at an IR zero of  $\beta$  and determining how much they shift the location of the zero. As was pointed out in [2], in general, a scheme transformation that is acceptable in the vicinity of the ultraviolet (UV) fixed point at  $\alpha = 0$  can produce unphysical effects in the vicinity of an infrared fixed point. These include, for example, having an inverse that maps a (real, positive) coupling to a negative or complex value. A set of conditions that a scheme transformation must satisfy in order to be physically acceptable was given [2] and was shown to be rather restrictive at a generic IR zero of  $\beta$ . A simple example is provided by the one-parameter family of scheme transformations

$$a = \frac{\tanh(ra')}{r} \quad (2.4)$$

(dependent on a parameter  $r$ ), with inverse

$$a' = \frac{1}{2r} \ln\left(\frac{1+ra}{1-ra}\right). \quad (2.5)$$

For example, if  $r = 4\pi$ , then Eq. (2.4) is the scheme transformation  $\alpha = \tanh \alpha'$ , and Eq. (2.5) is its inverse,  $\alpha' = (1/2) \ln[(1+\alpha)/(1-\alpha)]$ . The scheme transformation (2.4) is acceptable for small  $\alpha$  and hence  $a$ , but if  $a > 1/r$  (i.e.,  $\alpha > 4\pi/r$ ), then the transformation (2.5) maps a physical  $\alpha$  to a complex, unphysical  $\alpha'$ , and hence is unacceptable.

In addition to the general field-theoretic interest in understanding the evolution of a gauge coupling as a function of Euclidean momentum scale, one of the motivations for understanding the effect of scheme transformations on the beta function that describes this is to provide further information from continuum calculations to combine with information obtained from lattice computations. Indeed, an intensive program of research is underway using simulations of lattice gauge theories to study the infrared properties of gauge theories with multiple fermions in various representations of the gauge group [27]. In this context, it has been useful to compare results from higher-loop continuum calculations with lattice measurements, e.g. on the anomalous dimension of the fermion bilinear operator,  $\gamma_m(\alpha)$  evaluated at  $\alpha_{\text{IR}}$ , making use of the higher-loop calculations of this IR zero of  $\beta$  in [22,23]. In the chirally symmetric IR phase, a hypothetical all-orders calculation of  $\gamma_m$  evaluated at an all-orders calculation of  $\alpha_{\text{IR}}$  would be an exact property of the theory, while in the phase with spontaneous chiral symmetry breaking, just as the IR zero of  $\beta$  is only an approximate IR fixed point, so also,  $\gamma_m$  is only approximate, describing the running of

$\bar{\psi}\psi$  and the dynamically generated fermion mass near the zero of  $\beta$ . In both the chirally symmetric and chirally broken phases, one necessarily encounters the issue of scheme dependence in the calculation of both  $\alpha_{\text{IR}}$  and  $\gamma_m$  evaluated at  $\alpha = \alpha_{\text{IR}}$  at a finite loop order  $\ell \geq 3$ . It is therefore necessary to understand as well as possible the effects of scheme transformations, in particular, the scheme transformation  $S_{R,m}$  that can remove terms in the  $\beta$  function from loop order  $\ell = 3$  to  $\ell = m + 1$ . We proceed to discuss these scheme transformations next.

### III. GENERAL FRAMEWORK FOR SCHEME TRANSFORMATIONS

A scheme transformation can be expressed as a mapping between  $\alpha$  and  $\alpha'$ , or equivalently,  $a$  and  $a'$ , which we write as  $a = a'f(a')$ . We will refer to  $f(a')$  as the scheme transformation function. To keep the UV properties the same, one requires that  $f(0) = 1$ . We will consider  $f(a')$  that are analytic about  $a = a' = 0$  and hence can be expanded in the form

$$f(a') = 1 + \sum_{s=1}^{s_{\text{max}}} k_s (a')^s = 1 + \sum_{s=1}^{s_{\text{max}}} \bar{k}_s (\alpha')^s, \quad (3.1)$$

where the  $k_s$  are constants,  $\bar{k}_s = k_s/(4\pi)^s$ , and, *a priori*,  $s_{\text{max}}$  may be finite or infinite. From Eq. (3.1), it follows that the Jacobian  $J = da/da' = d\alpha/d\alpha'$  satisfies  $J = 1$  at  $a = a' = 0$ . After the scheme transformation is applied, the beta function in the new scheme has the form (2.2) with a new set of coefficients,  $b'_\ell$ ,

$$\beta_{\alpha'} \equiv \frac{d\alpha'}{dt} = \frac{d\alpha'}{d\alpha} \frac{d\alpha}{dt} = J^{-1} \beta_\alpha, \quad (3.2)$$

with the expansion

$$\beta_{\alpha'} = -2\alpha' \sum_{\ell=1}^{\infty} b'_\ell (\alpha')^\ell = -2\alpha' \sum_{\ell=1}^{\infty} \bar{b}'_\ell (\alpha')^\ell, \quad (3.3)$$

where  $\bar{b}'_\ell = b'_\ell/(4\pi)^\ell$ . One can then solve for the  $b'_\ell$  in terms of the  $b_\ell$  and  $k_s$ . This yields the known results that  $b'_1 = b_1$  and  $b'_2 = b_2$  [6], and the new results for  $b'_\ell$  at higher-loop order  $\ell$  that were presented in [2]. Since we will use these higher-loop results for our present work, we give a relevant list of them in Appendix A. It should be noted 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 scheme,  $b_2$  is actually gauge-dependent [28] and is not equal to  $b_2$  in the  $\overline{\text{MS}}$  scheme. We restrict our analysis here to gauge-invariant scheme transformations and to schemes, such as  $\overline{\text{MS}}$ , where  $b_2$  is independent of the gauge parameter. Here, as usual, by gauge invariance, we mean independence of the gauge parameter of the gauge-fixing term introduced in the quantization of the theory.

The  $n$ -loop beta function in the transformed scheme,  $\beta_{\alpha',n\ell}$ , is given by Eq. (3.3) with the upper limit on the  $\ell$

summation equal to  $n$  rather than  $\infty$ . It is also convenient to define two reduced beta functions with respective quadratic prefactors extracted, as in our earlier work, namely

$$\beta_{\alpha,n\ell,r} \equiv -\frac{\beta_{\alpha,n\ell,r}}{2\alpha^2} = \sum_{\ell=1}^n \bar{b}_\ell \alpha^{\ell-1} = \frac{1}{4\pi} \sum_{\ell=1}^n b_\ell \alpha^{\ell-1} \quad (3.4)$$

and similarly

$$\beta_{\alpha',n\ell,r} \equiv -\frac{\beta_{\alpha',n\ell,r}}{2\alpha'^2} = \sum_{\ell=1}^n \bar{b}'_\ell (\alpha')^{\ell-1} = \frac{1}{4\pi} \sum_{\ell=1}^n b'_\ell (\alpha')^{\ell-1}. \quad (3.5)$$

In order to be physically acceptable, a scheme transformation must satisfy several necessary conditions [2]. The first (denoted  $C_1$ ) is that 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 generically violate the unitarity of the theory. Second, as condition  $C_2$ , 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. Third, as condition  $C_3$ , the Jacobian  $J$  should not vanish in the region of  $\alpha$  and  $\alpha'$  of interest, or else there would be a pole in Eq. (3.2). 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  $b_2 < 0$ . Therefore, as the fourth condition,  $C_4$ , a scheme transformation should satisfy the property that  $\beta_\alpha$  has an IR zero if and only if  $\beta_{\alpha'}$  has an IR zero. Clearly, these conditions apply for both a scheme transformation and its inverse. The conditions can easily be satisfied by scheme transformations applied in the vicinity of a UV fixed point at small  $\alpha$ , but they are not automatically satisfied, and are a significant restriction, on a scheme transformation applied in the vicinity of a generic IR fixed point.

#### IV. SCHEME TRANSFORMATIONS $S_{R,m}$ AND $S_{R,\infty}$

In approaching the task of constructing a scheme transformation that maps an arbitrary initial scheme to the 't Hooft scheme, it is natural to begin by constructing a family of transformations such that the first removes the three-loop term in  $\beta_{\alpha'}$ , i.e., renders  $b'_3 = 0$ , the next renders  $b'_\ell = 0$  for  $\ell = 3$  and  $\ell = 4$ , and so forth. We thus define a scheme transformation  $S_{R,m}$  with  $s_{\max} = m$  and  $m \geq 2$  with the property that it removes terms in  $\beta_{\alpha'}$  from loop order 3 to loop order  $m + 1$ , inclusive. That is, starting from an arbitrary initial scheme and applying the scheme transformation  $S_{R,m}$ , one has, for the coefficients in the transformed scheme,

$$S_{R,m} \Rightarrow b'_\ell = 0 \quad \text{for } \ell = 3, \dots, m + 1. \quad (4.1)$$

Equivalently,  $S_{R,m}$  produces the  $n$ -loop beta function  $\beta_{\alpha',n\ell}$  in the transformed scheme

$$\begin{aligned} \beta_{\alpha',n\ell} &= -8\pi(a')^2 \left[ b_1 + b_2 a' + \sum_{\ell=m+2}^n b'_\ell (a')^{\ell-1} \right] \\ &= -2(\alpha')^2 \left[ \bar{b}_1 + \bar{b}_2 \alpha' + \sum_{\ell=m+2}^n \bar{b}'_\ell (\alpha')^{\ell-1} \right] \end{aligned} \quad (4.2)$$

and the full beta function  $\beta_{\alpha'} \equiv \lim_{n \rightarrow \infty} \beta_{\alpha',n\ell}$ . In Eq. (4.2) and in analogous equations below, it is understood implicitly that if  $n < m + 2$ , the terms involving sums over loop order from  $\ell = m + 2$  to  $\ell = n$  are to be replaced by zero.

There is a unique type of scheme transformation  $S_{R,m}$  that satisfies the properties that (i)  $b'_\ell = 0$  for  $\ell = 3, \dots, m + 1$ ; (ii) it has unique solutions for all of the  $m$  coefficients  $k_s$ ,  $s = 1, \dots, m$ , which, in turn, means that these coefficients are solutions of linear equations. The construction of this scheme uses the fact that the coefficient  $b'_\ell$  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 uniquely. To construct  $S_{R,m}$ , we take the simplest case,  $k_1 = 0$ . Using Eq. (A1) and solving the equation  $b'_3 = 0$  for  $k_2$ , we obtain  $k_2 = b_3/b_1$ , so

$$k_2 = \frac{b_3}{b_1} \quad \text{for } S_{R,m} \quad \text{with } m \geq 2. \quad (4.3)$$

If we only want to construct  $S_{R,2}$ , removing the three-loop term in  $\beta_{\alpha'}$ , this suffices. If we want to construct  $S_{R,m}$  with  $m \geq 3$ , removing at least the three-loop and four-loop terms in  $\beta_{\alpha'}$ , then we need to calculate  $k_3$ . To do this, we substitute these values of  $k_1$  and  $k_2$  into the expression in Eq. (A2) for  $b'_4$  and solve the equation  $b'_4 = 0$  for  $k_3$ , obtaining

$$k_3 = \frac{b_4}{2b_1} \quad \text{for } S_{R,m} \quad \text{with } m \geq 3. \quad (4.4)$$

To calculate the coefficient  $k_4$  needed for  $S_{R,m}$  with  $m \geq 4$ , we substitute the above values of  $k_s$  with  $s = 1, 2, 3$  into the expression in Eq. (A3) for  $b'_5$  and solve the equation  $b'_5 = 0$  for  $k_4$ . From this we find that

$$k_4 = \frac{b_5}{3b_1} - \frac{b_2 b_4}{6b_1^2} + \frac{5b_3^2}{3b_1^2} \quad \text{for } S_{R,m} \quad \text{with } m \geq 4. \quad (4.5)$$

To construct  $S_{R,m}$  for higher  $m$ , we continue iteratively in this manner. With the set of  $k_s$  coefficients calculated up to order  $s = m - 1$ , we calculate  $k_m$  by substituting the solutions for  $k_s$ ,  $s = 1, \dots, m - 1$ , into our expression for  $b'_{m+1}$ , then set  $b'_{m+1} = 0$ , and solve for  $k_m$ . We list the resultant  $k_s$  for  $s = 5, 6, 7$  in Appendix B. As is clear from this procedure and from the property that  $S_{R,m}$  involves coefficients  $k_s$  with  $s = 2, \dots, m$ , the explicit construction of the scheme transformation  $S_{R,m}$  in terms of the  $b_\ell$  coefficients of the  $\beta_\alpha$  function in an initial scheme requires

a knowledge of the  $b_\ell$  in this initial scheme up to the loop order  $\ell = m + 1$ . Since  $s_{\max} = m$  for  $S_{R,m}$ ,

$$k_s = 0 \quad \text{for } S_{R,m} \quad \text{if } s > m. \quad (4.6)$$

Using the set of coefficients  $k_s$  with  $k_1 = 0$  and  $k_s$ ,  $s = 2, \dots, m$  as calculated in Eqs. (4.3), (4.4), and (4.5) and iteratively for higher  $m$ , we define the transformation function  $f(a')$  for the scheme transformation  $S_{R,m}$ :

$$f(a')_{S_{R,m}} = 1 + \sum_{s=2}^m k_s (a')^s. \quad (4.7)$$

Applying this to an initial scheme, we obtain  $b'_\ell = 0$  for  $\ell = 3, \dots, m + 1$ , as in (4.1) and (4.2).

Some remarks on structural properties of these  $k_s$  coefficients are in order. The coefficient  $k_s$  depends on the  $b_\ell$  with  $\ell = 1, \dots, s + 1$  via the ratios

$$\frac{b_\ell}{b_1}, \quad \text{for } \ell = 2, \dots, s + 1. \quad (4.8)$$

It follows that these  $k_s$  have the property

$$k_s \text{ is invariant under the rescaling } b_\ell \rightarrow \lambda b_\ell, \quad (4.9)$$

where  $\lambda \in \mathbb{R}$ . A corollary is that

$$S_{R,m} \text{ is invariant under the rescaling } b_\ell \rightarrow \lambda b_\ell. \quad (4.10)$$

Since  $S_{R,m}$  requires knowledge of the  $b_\ell$  up to loop order  $\ell = m + 1$  and since the  $b_\ell$  have been calculated up to  $\ell = 4$  loops for a general non-Abelian gauge theory [13,14], it follows that the highest order for which we can calculate and apply the  $S_{R,m}$  scheme transformation is  $m = 3$ .

A scheme transformation that can map an arbitrary initial scheme to a scheme in which the beta function consists only of the one-loop and two-loop terms necessarily has  $s_{\max} = \infty$ , since it must remove  $m$ -loop coefficients up to arbitrarily high order. We define  $S_{R,\infty} = \lim_{m \rightarrow \infty} S_{R,m} \equiv S_H$ . The transformation  $S_{R,\infty}$  fulfills the purpose of mapping an arbitrary initial scheme to a scheme in which  $b'_\ell = 0$  for all  $\ell \geq 3$ , so that the resultant beta function is reduced to just the (scheme-independent) one-loop and two-loop terms, i.e.,

$$S_{R,\infty} \Rightarrow \beta_{\alpha'} = -8\pi a^2 (b_1 + b_2 a) = -2\alpha^2 (\bar{b}_1 + \bar{b}_2 \alpha). \quad (4.11)$$

Since the application of the scheme transformation  $S_{R,m}$  to an arbitrary initial scheme produces a  $\beta_{\alpha'}$  function with  $b'_\ell = 0$  for  $\ell = 3, \dots, m + 1$ , as expressed in Eqs. (4.1) and (4.2), it follows that in the new scheme, the IR zero of the  $n$ -loop beta function  $\beta_{\alpha',n\ell}$  is at the same value as the (scheme-independent) value  $\alpha_{\text{IR},2\ell}$  for  $n$  up to and including  $n = m + 1$ , i.e.,

$$S_{R,m} \Rightarrow \alpha'_{\text{IR},n\ell} = \alpha_{\text{IR},2\ell} \quad \text{for } n = 3, \dots, m + 1. \quad (4.12)$$

## V. COEFFICIENTS $b'_\ell$ RESULTING FROM $S_{R,m}$ SCHEME TRANSFORMATION

### A. $S_{R,2}$

For our applications, it will be useful to exhibit the explicit results for the coefficients  $b'_\ell$  resulting from the applications of the scheme transformations  $S_{R,m}$  with  $m = 2, 3, 4$ . In this subsection we show these for the case  $m = 2$ . Substituting the relevant  $k_s$  for the  $S_{R,2}$  scheme in the general expressions for the  $b'_\ell$ , we find

$$b'_3 = 0, \quad (5.1)$$

$$b'_4 = b_4, \quad (5.2)$$

$$b'_5 = b_5 + \frac{5b_3^2}{b_1}, \quad (5.3)$$

$$b'_6 = b_6 + \frac{2b_3b_4}{b_1} + \frac{3b_2b_3^2}{b_1^2}, \quad (5.4)$$

$$b'_7 = b_7 + \frac{3b_3b_5}{b_1} - \frac{9b_3^3}{b_1^3}, \quad (5.5)$$

$$b'_8 = b_8 + \frac{4b_3b_6}{b_1} + \frac{4b_3^2b_4}{b_1^2} - \frac{8b_2b_3^3}{b_1^3}. \quad (5.6)$$

In general, after the  $S_{R,2}$  scheme transformation is applied, the resultant  $n$ -loop beta function,  $\beta_{\alpha',n\ell}$ , has the form of Eq. (4.2) with  $m = 2$ .

### B. $S_{R,3}$

From the expressions for  $k_s$  in the  $S_{R,3}$  scheme transformation, we calculate the resultant  $b'_\ell$  coefficients. We obtain

$$b'_3 = b'_4 = 0, \quad (5.7)$$

$$b'_5 = b_5 + \frac{5b_3^2}{b_1} - \frac{b_2b_4}{2b_1}, \quad (5.8)$$

$$b'_6 = b_6 + \frac{8b_3b_4}{b_1} + \frac{3b_2b_3^2}{b_1^2}, \quad (5.9)$$

$$b'_7 = b_7 + \frac{3b_3b_5}{b_1} + \frac{11b_4^2}{4b_1} - \frac{9b_3^3}{b_1^3} + \frac{9b_2b_3b_4}{2b_1^2}, \quad (5.10)$$

$$b'_8 = b_8 + \frac{4b_3b_6}{b_1} + \frac{b_4b_5}{b_1} - \frac{18b_3^2b_4}{b_1^2} + \frac{7b_2b_4^2}{4b_1^2} - \frac{8b_2b_3^3}{b_1^3}. \quad (5.11)$$

After the  $S_{R,3}$  scheme transformation is applied,  $\beta_{\alpha',n\ell}$  has the form of Eq. (4.2) with  $m = 3$ .

We give the corresponding results for the coefficients  $b'_\ell$  resulting from the scheme transformation  $S_{R,4}$  in Appendix C.

## VI. APPLICATION OF THE $S_{R,2}$ SCHEME TRANSFORMATION

As a foundation for our analysis of the scheme transformation  $S_{R,3}$ , we recall our results from [2] concerning  $S_{R,2}$  (denoted as  $S_2$  in [2]). Let us consider an asymptotically free gauge theory with gauge group  $G$  and  $N_f$  massless fermions in a representation  $R$  of  $G$ . Since [7,29]

$$b_1 = \frac{1}{3}(11C_A - 4T_f N_f), \quad (6.1)$$

the property of asymptotic freedom implies that  $N_f < N_{f,b1z}$ , where [30]

$$N_{f,b1z} = \frac{11C_A}{4T_f}. \quad (6.2)$$

The two-loop coefficient is [8,9]

$$b_2 = \frac{1}{3}[34C_A^2 - 4(5C_A + 3C_f)T_f N_f], \quad (6.3)$$

which decreases monotonically with increasing  $N_f$  and reverses sign as  $N_f$  increases through  $N_{f,b2z}$ , where

$$N_{f,b2z} = \frac{34C_A^2}{4(5C_A + 3C_f)T_f}. \quad (6.4)$$

Now for arbitrary  $G$  and  $R$ ,

$$N_{f,b2z} < N_{f,b1z}, \quad (6.5)$$

as is evident from the fact that the difference,

$$N_{f,b1z} - N_{f,b2z} = \frac{3C_A(11C_f + 7C_A)}{4T_f(3C_f + 5C_A)} > 0. \quad (6.6)$$

Hence, there is always an interval in  $N_f$  such that  $b_1 > 0$  while  $b_2 < 0$ , so that the two-loop ( $2\ell$ ) beta function has an IR zero. We denote this interval as  $I$ :

$$I: N_{f,b2z} < N_f < N_{f,b1z}. \quad (6.7)$$

The zero of the two-loop beta function (which is scheme independent) occurs at  $\alpha = \alpha_{\text{IR},2\ell}$ , where

$$\alpha_{\text{IR},2\ell} = -\frac{4\pi b_1}{b_2} \quad (6.8)$$

(i.e.,  $\alpha_{\text{IR},2\ell} = -b_1/b_2$ ), which is physical for  $N_f \in I$ . From the  $m = 2$  special case of Eq. (4.12), it follows that after the application of the  $S_{R,2}$  scheme transformation, in terms of the new variable  $\alpha'$ ,

$$\alpha'_{\text{IR},3\ell} = \alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell}. \quad (6.9)$$

For the  $S_{R,2}$  scheme transformation, the function  $f(a')$  has the form

$$S_{R,2}: f(a') = 1 + \frac{b_3}{b_1}(a')^2 = 1 + \frac{\bar{b}_3}{\bar{b}_1}(a')^2. \quad (6.10)$$

Now we assume that  $N_f \in I$ , so that there is an IR zero in  $\beta_{2\ell}$ , as given in Eq. (6.8). We start in the  $\overline{\text{SM}}$  scheme and operate with the  $S_{R,2}$  scheme transformation. We evaluate  $f(a')$  at this IR zero,  $\alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell} = -b_1/b_2$  and obtain the following result:

$$S_{R,2}: f(\alpha'_{\text{IR},2\ell}) = 1 + \frac{b_1 b_3}{b_2^2} = 1 + \frac{\bar{b}_1 \bar{b}_3}{\bar{b}_2^2}. \quad (6.11)$$

In order that this transformation obey condition  $C_1$ , namely that it maps  $a' > 0$  to  $a > 0$ , we require that  $f(a') > 0$ . This inequality must be satisfied, in particular, at  $\alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell}$ , so we obtain the inequality

$$1 + \frac{\bar{b}_1 \bar{b}_3}{\bar{b}_2^2} > 0. \quad (6.12)$$

Since  $\bar{b}_3 < 0$  for  $N_f \in I$  in the  $\overline{\text{MS}}$  scheme, and, more generally, in schemes that maintain at the three-loop level the IR zero in the two-loop beta function [25], we can also write this in terms of positive quantities as the condition that

$$1 - \frac{\bar{b}_1 |\bar{b}_3|}{\bar{b}_2^2} > 0. \quad (6.13)$$

This analysis holds for an arbitrary gauge group  $G$  and fermion content such that the two-loop  $\beta$  function has an IR zero.

As was shown in [2], the inequality (6.12) is not, in general, satisfied, so this  $S_{R,2}$  scheme transformation violates condition  $C_1$  in the vicinity of the IR fixed point for a certain range of smaller values of  $N_f \in I$ . To show the violation of the inequality (6.12), it suffices to consider the class of theories with  $G = \text{SU}(N_c)$  and  $N_f$  fermions in the fundamental representation. The interval  $I$  where the two-loop  $\beta$  function has an IR zero is then

$$I: \frac{34N_c^3}{13N_c^2 - 3} < N_f < \frac{11N_c}{2}. \quad (6.14)$$

For  $N_c = 2$ , the interval  $I$  is  $5.55 < N_f < 11$ , while for  $N_c = 3$ ,  $I$  is  $8.05 < N_f < 16.5$ . For  $N_c = 2$ , the inequality (6.12) is violated for  $5.55 < N_f < 8.44$  and is satisfied for  $8.44 < N_f < 11$ , while for  $N_c = 3$ , inequality is violated for  $8.05 < N_f < 12.41$  and is satisfied for  $12.41 < N_f < 16.5$ . Note that the same is true if  $f(a')$  is evaluated for  $a' = \alpha'_{\text{IR},3\ell}$ , since by Eq. (4.12),  $\alpha'_{\text{IR},3\ell} = \alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell}$ . In Table I of [2] we gave the values of  $\alpha'_{\text{IR},4\ell}$  resulting from the application of the  $S_{R,2}$  scheme transformation. In Table I of the present paper we list the values of  $f(\alpha'_{\text{IR},2\ell})$  for this  $S_{R,2}$  scheme transformation, for the illustrative values  $2 \leq N_c \leq 4$  and  $N_f$  in the respective intervals  $I$  for each  $N_c$ . Given a value of  $N_c$ , for values of  $N_f$  near the lower end of the respective interval  $I$ ,  $|f(a')|$  gets large compared to unity. This is a consequence of the fact that

TABLE I. Values of  $S_{R,n}$  scheme transformation function  $f(a')$ , evaluated at the scheme-independent value of the two-loop IR zero,  $a'_{\text{IR},2\ell} = a_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell}/(4\pi)$ , denoted  $f(a')_{\text{IR},S_{R,n}}$ . We list results for  $S_{R,n}$  with  $n = 2$  and  $n = 3$  in the  $\text{SU}(N_c)$  gauge theory with  $2 \leq N_c \leq 4$  and with  $N_f$  fermions transforming according to the fundamental representation, as functions of  $N_c$  and  $N_f$ , for values of  $N_f$  in the respective intervals  $I$  where the theory is asymptotically free and the two-loop beta function  $\beta_{2\ell}$  has an infrared zero.

$N_c$	$N_f$	$\alpha_{\text{IR},2\ell}$	$f(a')_{\text{IR},S_{R,2}}$	$f(a')_{\text{IR},S_{R,3}}$
2	7	2.83	-3.529	-1.898
2	8	1.26	-0.5075	-0.154
2	9	0.595	0.399	0.497
2	10	0.231	0.795	0.813
3	10	2.21	-4.454	-3.335
3	11	1.23	-1.418	-0.921
3	12	0.754	-0.272	-0.027
3	13	0.468	0.293	0.412
3	14	0.278	0.616	0.667
3	15	0.143	0.818	0.833
3	16	0.0416	0.9505	0.952
4	13	1.85	-5.333	-4.463
4	14	1.16	-2.243	-1.668
4	15	0.783	-0.912	-0.548
4	16	0.546	-0.204	-0.0207
4	17	0.384	0.221	0.355
4	18	0.266	0.498	0.573
4	19	0.175	0.688	0.726
4	20	0.105	0.825	0.840
4	21	0.0472	0.925	0.928

$b_2 \rightarrow 0$  at this lower boundary of the interval  $I$  and hence formally,  $\alpha_{\text{IR},2\ell}$  diverges. Thus, for these values of  $N_f$ , in addition to the fact that this  $S_{R,2}$  scheme transformation violates condition  $C_1$  because  $f(a')$  is negative, it also violates condition  $C_4$ , because it maps moderate values of the gauge coupling to values that are too large for perturbation theory to be reliable.

## VII. APPLICATION OF THE $S_{R,3}$ SCHEME TRANSFORMATION

We next address and answer the question of whether one can alleviate or circumvent the pathology encountered with  $S_{R,2}$  at an IR fixed point [negative  $f(a')$  for various  $N_f \in I$ ] by instead using  $S_{R,3}$ . The transformation function  $f(a')$  for  $S_{R,3}$  is

$$\begin{aligned}
S_{R,3}: f(a') &= 1 + k_2(a')^2 + k_3(a')^3 \\
&= 1 + \frac{b_3}{b_1}(a')^2 + \frac{b_4}{2b_1}(a')^3 \\
&= 1 + \frac{\bar{b}_3}{\bar{b}_1}(\alpha')^2 + \frac{\bar{b}_4}{2\bar{b}_1}(\alpha')^3. \quad (7.1)
\end{aligned}$$

From the  $m = 3$  special case of Eq. (4.12), it follows that after the application of the  $S_{R,3}$  scheme transformation, in terms of the new variable  $\alpha'$ ,

$$\alpha'_{\text{IR},4\ell} = \alpha'_{\text{IR},3\ell} = \alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell}. \quad (7.2)$$

We use the same technique as for the analysis of  $S_{R,2}$ , namely we consider  $N_f \in I$ , so that  $\beta_{2\ell}$  has an IR zero. Evaluating  $f(a')$  at this (scheme-independent) two-loop zero,  $a'_{\text{IR},2\ell} = a_{\text{IR},2\ell} = -b_1/b_2$ , we have

$$f(a'_{\text{IR},2\ell}) = 1 + \frac{b_1 b_3}{b_2^2} - \frac{b_1^2 b_4}{2b_2^3} = 1 + \frac{\bar{b}_1 \bar{b}_3}{\bar{b}_2^2} - \frac{\bar{b}_1^2 \bar{b}_4}{2\bar{b}_2^3}. \quad (7.3)$$

In order for the  $S_{R,3}$  scheme transformation to be acceptable, a necessary condition is  $C_1$ , that  $f(a') > 0$ , in particular, at  $a' = a_{\text{IR},2\ell} = a_{\text{IR},2\ell}$ , i.e., that

$$1 + \frac{\bar{b}_1 \bar{b}_3}{\bar{b}_2^2} - \frac{\bar{b}_1^2 \bar{b}_4}{2\bar{b}_2^3} > 0. \quad (7.4)$$

Now  $b_2 < 0$  for  $N_f \in I$  and, as shown in [25]  $b_3 < 0$  for  $N_f \in I$  not only in the  $\overline{\text{MS}}$  scheme, but more generally in any scheme that has the necessary property of maintaining the scheme-independent property that the two-loop  $\beta$  function has an IR zero. Given these properties, we can reexpress (7.4) in terms of positive quantities as

$$1 - \frac{\bar{b}_1 |\bar{b}_3|}{\bar{b}_2^2} + \frac{\bar{b}_1^2 \bar{b}_4}{2|\bar{b}_2|^3} > 0. \quad (7.5)$$

As is evident in Table I of [22], for  $N_c = 2$  and  $N_c = 3$ ,  $b_4$  is positive for all  $N_f$  in the respective intervals  $I$ , but for  $N_c \geq 4$ ,  $b_4$  can be negative for some value(s) of  $N_f \in I$ .

This analysis for  $S_{R,3}$  holds for an arbitrary gauge group  $G$  and fermion representation such that  $N_f \in I$ . For our present purposes, it will suffice to consider the case  $G = \text{SU}(N_c)$  and fermions in the fundamental representation. As before, we start in the  $\overline{\text{MS}}$  scheme. In Table I we list values of  $f(a'_{\text{IR},2\ell})$  for the  $S_{R,3}$  scheme transformation, for  $N_c = 2, 3, 4$  and  $N_f$  in the respective intervals  $I$  for each  $N_c$  where the two-loop beta function has an IR zero. As we noted above in the case of  $S_{R,2}$ , for smaller values of  $N_f$  in the respective interval  $I$  for each  $N_c$ ,  $|f(a')|$  is substantially larger than unity, so that, in addition to the violation of condition  $C_1$ ,  $f(a')$  also violates condition  $C_4$ . We omit entries for the lowest values of  $N_f$  in the respective intervals  $I$ , for which  $|f(a')| \gg 1$ , where this violation is most extreme, for example, for  $\text{SU}(3)$  with  $N_f = 9$ ,  $f(a')_{\text{IR},S_{R,2}} = -19.851$ , and  $f(a')_{\text{IR},S_{R,3}} = -15.282$ .

From our Table I, one sees that for  $N_c = 2, 3, 4$ , the values of  $N_f$  that yield an unphysical negative  $f(a')$  for the  $S_{R,2}$  scheme transformation also yield an unphysical negative  $f(a')$  for the  $S_{R,3}$  scheme transformation. This is also true for almost all of the values of  $N_f$  in the case  $N_c = 5$ , with one exception; for  $N_f = 20$ ,  $f(a_{\text{IR},2\ell}) < 0$  for  $S_{R,2}$ ,

while  $f(a_{\text{IR},2\ell}) > 0$  for  $S_{R,3}$ . We have also investigated this for higher  $N_c$ , with similar findings. We note that the same results are obtained by substituting the three-loop IR zero, since by Eq. (4.12) this is equal to the scheme-independent two-loop IR zero. Therefore, using the  $S_{R,3}$  scheme transformation does not alleviate the problem encountered with the  $S_{R,2}$  transformation and does not significantly increase the range of  $N_f$  where  $f(a')$  satisfies the necessary condition of being positive when evaluated at the scheme-independent value  $a_{\text{IR},2\ell}$ . These  $S_{R,m}$  scheme transformations can be used for larger values of  $N_f$  toward the upper end of the interval  $I$ , where  $\alpha_{\text{IR},2\ell}$  is correspondingly smaller, approaching zero as  $N_f \nearrow N_{f,b1z}$ . However, to show this for  $S_{R,\infty}$  is delicate, since it requires that one analyze the convergence of an infinite series [2].

In passing, we remark on a related topic. For this purpose, let us consider a general (vectorial) gauge theory with an arbitrary non-Abelian gauge group  $G$  and  $N_f$  fermions in an arbitrary representation. For a given  $G$  and  $R$ , let us consider increasing  $N_f$  past the value where  $b_1$  reverses sign, so that the theory becomes nonasymptotically free. One may ask whether this theory has an ultraviolet fixed point and if so, what is the range of applicability of the  $S_{R,m}$  scheme transformation for various  $m$ . Because of the inequality (6.5), it follows that if  $N_f > N_{f,b1z}$  (so  $b_1 < 0$ ), then also  $N_f > N_{f,b2z}$ , so that  $b_2 < 0$ . Hence, this theory has no two-loop zero in its  $\beta$  function. Since this is the maximal scheme-independent information that one has, even if one were to obtain a zero of the  $\beta$  function at higher loops (which would now be a UV fixed point), one could not convincingly argue that this is physical. Below we shall discuss this sort of question further for a UV zero in the  $\beta$  function of a U(1) gauge theory.

### VIII. $S_{R,m}$ SCHEME TRANSFORMATION IN THE LIMIT $N_c \rightarrow \infty$ , $N_f \rightarrow \infty$ WITH $N_f/N_c$ FIXED

For the case of  $G = \text{SU}(N_c)$  and  $N_f$  fermions in the fundamental representation, a limit of particular interest is the 't Hooft-Veneziano limit [31],

$$N_c \rightarrow \infty, \quad N_f \rightarrow \infty, \quad \text{with } r \equiv \frac{N_f}{N_c} \text{ fixed.} \quad (8.1)$$

In this limit, one also requires that the product

$$\xi(\mu) \equiv \alpha(\mu)N_c \quad (8.2)$$

be a fixed, finite function of  $\mu$ . We denote this as the LNN (large  $N_c$  and  $N_f$ ) limit.

Here we investigate the applicability of the  $S_{R,2}$  and  $S_{R,3}$  scheme transformations for  $N_f \in I$  in the LNN limit. One of the reasons for the interest in the LNN limit is that properties of the  $\beta$  function exhibit an approximate universality, in the sense that they are similar for different values of  $N_c$  and  $N_f$  if the ratio  $r = N_f/N_c$  is similar or the

same [22,25]. The study in [26] gave some insight into the origin of this universality.

To construct an appropriate beta function that has a finite, nontrivial LNN limit, one multiplies both sides of Eq. (2.2) by  $N_c$  and then takes this limit, obtaining a result that is a function of  $\xi$ ,

$$\beta_\xi \equiv \frac{d\xi}{dt} = \lim_{\text{LNN}} \beta_a N_c. \quad (8.3)$$

This beta function has the expansion

$$\beta_\xi \equiv \frac{d\xi}{dt} = -8\pi x \sum_{\ell=1}^{\infty} \hat{b}_\ell x^\ell = -2\xi \sum_{\ell=1}^{\infty} \tilde{b}_\ell \xi^\ell, \quad (8.4)$$

where  $x = \xi/(4\pi)$  and

$$\hat{b}_\ell = \lim_{\text{LNN}} \frac{b_\ell}{N_c^\ell}, \quad \tilde{b}_\ell = \lim_{\text{LNN}} \frac{\bar{b}_\ell}{N_c^\ell}. \quad (8.5)$$

Thus,  $\tilde{b}_\ell = \hat{b}_\ell/(4\pi)^\ell$ . One defines the  $n$ -loop  $\beta_\xi$  function by Eq. (8.4) with the upper limit on the summation over loop order  $\ell = \infty$  replaced by  $\ell = n$ .

The (scheme-independent) one-loop and two-loop coefficients in  $\beta_\xi$  are

$$\hat{b}_1 = \frac{1}{3}(11 - 2r) \quad (8.6)$$

and

$$\hat{b}_2 = \frac{1}{3}(34 - 13r). \quad (8.7)$$

Asymptotic freedom requires that  $b_1 > 0$  and hence that  $r < 11/2$ . The coefficient  $\hat{b}_2$  reverses sign to negative values as  $r$  increases through the value  $r = 34/13$ . Consequently, for  $r$  in the real interval

$$I_r: \quad \frac{34}{13} < r < \frac{11}{2}, \quad (8.8)$$

i.e.,  $2.6154 < r < 5.5$ ,  $\beta_{\xi,2\ell}$  has an IR zero. This zero occurs at

$$\xi_{\text{IR},2\ell} = 4\pi x_{\text{IR},2\ell} = \frac{4\pi(11 - 2r)}{13r - 34}. \quad (8.9)$$

The three-loop and four-loop coefficients  $\hat{b}_3$  and  $\hat{b}_4$  were given in [26].

A scheme transformation applicable to the theory in the LNN limit is thus

$$x = x'f(x'). \quad (8.10)$$

One requires that  $f(0) = 1$  to keep the UV properties the same. Considering  $f(x')$  that are analytic at  $x' = x = 0$ , one has the expansion

$$f(x') = 1 + \sum_{s=1}^{s_{\text{max}}} k_s (x')^s = 1 + \sum_{s=1}^{s_{\text{max}}} \bar{k}_s (\xi')^s. \quad (8.11)$$



Evaluating the  $S_{R,2}$  expression for  $f(x')$  in the LNN limit at  $x = x_{\text{IR},2\ell}$ , we calculate

$$S_{R,2;\text{LNN}} \Rightarrow f(x')_{\text{IR},2\ell} = \frac{52235 - 40425r + 7692r^2 - 224r^3}{18(13r - 34)^2}. \quad (8.12)$$

For  $r \in I_r$ , this  $f(x')$  is a monotonically increasing function of  $r$ , which passes through zero from negative to positive values as  $r$  increases through the value  $r = 4.06814$  (quoted to the indicated accuracy). Thus,

$$\begin{aligned} S_{R,2;\text{LNN}} \Rightarrow f(x')_{\text{IR},2\ell} < 0 & \quad \text{for } 2.6154 < r < 4.0681 \\ f(x')_{\text{IR},2\ell} > 0 & \quad \text{for } 4.0681 < r < 5.5000. \end{aligned} \quad (8.13)$$

Evaluating the  $S_{R,3}$  expression for  $f(x')$  in the LNN limit at  $x = x_{\text{IR},2\ell}$ , we obtain

$$\begin{aligned} S_{R,3;\text{LNN}} \Rightarrow \\ f(x')_{\text{IR},2\ell} = \frac{1}{6^4(13r - 34)^3} & [-55042348 + 62622039r \\ & - 24520604r^2 + 2885644r^3 + 21504r^4 \\ & + 4160r^5 + \zeta(3)(1149984 - 940896r \\ & + 2423520r^2 - 815616r^3 + 72576r^4)]. \end{aligned} \quad (8.14)$$

Here,  $\zeta(s) \equiv \sum_{n=1}^{\infty} n^{-s}$  is the Riemann zeta function, with  $\zeta(3) = 1.202057$ , etc. For  $r \in I_r$ , this  $f(x')$  is again a monotonically increasing function of  $r$ , which passes through zero from negative to positive values as  $r$  increases through the value  $r = 3.95069$  (to the indicated accuracy). Thus,

$$\begin{aligned} S_{R,3;\text{LNN}} \Rightarrow f(x')_{\text{IR},2\ell} < 0 & \quad \text{for } 2.6154 < r < 3.9507 \\ f(x')_{\text{IR},2\ell} > 0 & \quad \text{for } 3.9507 < r < 5.5000. \end{aligned} \quad (8.15)$$

Evidently, the positivity properties of  $f(x')$  for the  $S_{R,2}$  and  $S_{R,3}$  scheme transformations are quite similar in this LNN limit. This is in agreement with our calculations in Table I for specific values of  $N_c$  and  $N_f$ . Clearly, in the respective intervals of  $r$  where  $f(x')$  is negative, the  $S_{R,2}$  and  $S_{R,3}$  scheme transformations are unacceptable, since they fail to satisfy the condition  $C_1$ .

## IX. U(1) GAUGE THEORY

### A. General

It is also of interest to explore the effects of higher-order terms and the associated scheme dependence in the  $\beta$  function for an Abelian gauge theory. We consider the simplest example of such a theory, namely a vectorial theory with a U(1) gauge group and  $N_f$  fermions of charge

$q$ . We use the same notation for the gauge coupling  $g(\mu)$  and for  $\alpha(\mu)$  and  $a(\mu) = \alpha(\mu)/(4\pi)$  as before. With no loss of generality, we absorb  $q$  into the definition of  $g$ . As is well known, this theory is not asymptotically free and must be regarded as a low-energy effective field theory. One may investigate whether the two-loop  $\beta$  function for this theory has a zero, which would thus be an exact or approximate ultraviolet fixed point (UVFP). If, indeed, such a UV zero were present in the  $\beta$  function, one could also study the effect of the  $S_{R,m}$  scheme transformation on its value. In contrast to the case of an IRFP in an asymptotically free theory, here the UV to IR evolution would be envisioned as starting from the UVFP and flowing to weaker coupling.

For convenience, we define  $\beta_\alpha$  for this theory without the minus sign prefactor in Eq. (2.2). The coefficients that have been calculated can be obtained from those for the non-Abelian theory by the formal replacements  $C_A = 0$ ,  $C_f = 1$ , and  $T_f = 1$ , together with replacements of other group invariants that enter at the four-loop level [14]. If one fixes  $\alpha(\mu)$  at a some high scale  $\mu = \Lambda$  in the ultraviolet, then for a U(1) gauge theory with fermions of negligibly small mass,  $\alpha(\mu) \rightarrow 0$  as  $\mu \rightarrow 0$ , so the theory becomes free in the infrared (often called the triviality property). Actually, because there is no confinement, a U(1) theory with exactly zero-mass charged fermions has problems with infrared divergences, so a more precise statement of this property is that for the U(1) theory with fermions of mass  $m_0 \ll \Lambda$ , the running coupling  $\alpha(m_0)$  becomes arbitrarily small as  $m_0/\Lambda \rightarrow 0$ . If one were to take  $\mu < m_0$ , then in the construction of the low-energy effective field theory applicable in this interval, one would integrate out the fermions, and thereby obtain a free theory. Viewed the other way, from the IR to the UV, if one fixes  $\alpha(\mu)$  at some scale in the infrared such as  $\mu = m_0$  and then increases  $\mu$ , a solution of the one-loop  $\beta$  function equation yields a Landau pole. Of course, the perturbative calculation that produces this result is not reliable when  $\alpha(\mu)$  becomes so large as to approach this pole. Moreover, this would not be relevant to the actual physics if the ultraviolet completion of the U(1) gauge theory involves embedding of the U(1) factor group in an asymptotically free simple non-Abelian gauge group, as is the case with the embedding of the weak hypercharge U(1)<sub>Y</sub> factor group in a grand unified theory. It may be recalled that among the motivations for grand unification, one is that this embedding provides an elegant explanation of the quantization of weak hypercharge and hence electric charge in the Standard Model.

A number of studies have been performed to investigate the properties of U(1) gauge theory with fermions using methods going beyond perturbation theory, such as approximate solutions of Schwinger-Dyson equations [32,33] and simulations of the theory on a lattice [33,34]. In particular, fully nonperturbative lattice studies were carried out with dynamical staggered fermions (effectively corresponding to  $N_f = 4$  continuum fermion species) and

led to the conclusion that this theory does not have a (nontrivial) UV fixed point [33,34]. This question has also been examined using analytic results for the large- $N_f$  limit of the theory [23,35]. For our present purposes, we focus on the specific question of the scheme dependence of a possible UV zero in  $\beta$ , as is manifested in the effects of higher-loop terms. This is timely in part because the five-loop term in  $\beta$  has recently been calculated, as discussed below.

### B. $\beta_{\alpha,2\ell}$

Given that for this U(1) gauge theory we define  $\beta_\alpha$  as in Eq. (2.2) but without the minus sign prefactor, the one-loop and two-loop coefficients are [4,36]

$$b_1 = \frac{4N_f}{3} \quad (9.1)$$

and

$$b_2 = 4N_f. \quad (9.2)$$

Because  $b_1$  and  $b_2$  have the same sign, the two-loop  $\beta$  function,  $\beta_{\alpha,2\ell}$ , for this U(1) theory does not have a UV zero. As noted above, the two-loop beta function embodies the maximal scheme-independent information on the coupling constant evolution of the theory. Of course, this analysis is within the context of the perturbatively calculated  $\beta$  function and does not address the possibility of a nonperturbative UV zero. Owing to the absence of a UV zero in the two-loop  $\beta$  function, we cannot use the same method that we employed above to test the applicability of a scheme transformation, namely to evaluate  $f(a')$  at the two-loop zero and check to see where it is positive and of moderate size. Consequently, in order to study scheme-dependent effects in the context of a possible UV zero in the  $\beta$  function, we will simply investigate whether, for a given  $N_f$ , the higher-loop terms in  $\beta$  lead to a UV zero, and, if so, how the location of this zero changes as a function of loop order. Because of the absence of a UV zero in  $\beta$  at the two-loop level, even where it is present at the scheme-dependent higher-loop order, this perturbative analysis does not yield convincing evidence that it is physical.

### C. $\beta_{\alpha,3\ell}$

In the  $\overline{\text{MS}}$  scheme, the three-loop coefficient in the  $\beta$  function of the U(1) gauge theory has the negative-definite value [37,38]

$$b_3 = -2N_f \left( 1 + \frac{22N_f}{9} \right), \quad (9.3)$$

so that the three-loop beta function is

$$\beta_{\alpha,3\ell} = 8\pi N_f a^2 \left[ \frac{4}{3} + 4a - 2 \left( 1 + \frac{22N_f}{9} \right) a^2 \right]. \quad (9.4)$$

Thus, in addition to the IR zero at  $\alpha = 0$ , in the  $\overline{\text{MS}}$  scheme,  $\beta_{\alpha,3\ell}$  vanishes at the UV zero

$$\alpha_{\text{UV},3\ell} = 4\pi a_{\text{UV},3\ell} = \frac{4\pi \left[ 9 + \sqrt{3(45 + 44N_f)} \right]}{9 + 22N_f} \quad (9.5)$$

(and, formally, at an unphysical negative value of  $a$  given by the above expression with a minus sign in front of the square root). We list values of  $\alpha_{\text{UV},3\ell}$  in Table II as a function of  $N_f$  for  $N_f = 1$  to  $N_f = 10$ .

From Eq. (9.5), it follows that, in the  $\overline{\text{MS}}$  scheme, this  $\alpha_{\text{UV},3\ell}$  is a monotonically decreasing function of  $N_f$ . As  $N_f \rightarrow \infty$ ,  $\alpha_{\text{UV},3\ell}$  approaches zero like

$$\alpha_{\text{UV},3\ell} = 4\pi \sqrt{\frac{3}{11N_f}} \left[ 1 + \frac{3}{22} \sqrt{\frac{33}{N_f}} + \frac{9}{88N_f} + O\left(\frac{1}{(N_f)^{3/2}}\right) \right]. \quad (9.6)$$

Note that, even apart from the scheme dependence, for moderate  $N_f$ , the value of  $\alpha_{\text{UV},3\ell}$  in Eq. (9.5) is too large for the perturbative three-loop calculation to be very accurate. The fact that  $\alpha_{\text{UV},3\ell} \sim O(1)$  means that higher-loop corrections are generically important. We turn next to these.

### D. $\beta_{\alpha,4\ell}$

In the  $\overline{\text{MS}}$  scheme the four-loop coefficient in the  $\beta$  function of the U(1) gauge theory is [15,39]

$$b_4 = N_f \left[ -46 + \left( \frac{760}{27} - \frac{832}{9} \zeta(3) \right) N_f - \frac{1232}{243} N_f^2 \right]. \quad (9.7)$$

Numerically,

$$b_4 = -N_f (46 + 82.97533N_f + 5.06996N_f^2). \quad (9.8)$$

Evidently,  $b_4 < 0$  for all  $N_f > 0$ . The condition that  $\beta_{\alpha,4\ell} = 0$  for  $\alpha \neq 0$ , is the cubic equation in  $\alpha$ , or

TABLE II. Values of the UV zero in the  $\beta$  function of the U(1) gauge theory with  $N_f$  fermions, at  $n$ -loop ( $n\ell$ ) order, for  $n = 3, 4, 5$ , in the  $\overline{\text{MS}}$  scheme, denoted  $\alpha_{\text{UV},n\ell}$ . The symbol  $-$  indicates that there is no zero in  $\beta$  for the given order and value of  $N_f$ . See text for further details.

$N_f$	$\alpha_{\text{UV},3\ell}$	$\alpha_{\text{UV},4\ell}$	$\alpha_{\text{UV},5\ell}$
1	10.2720	3.0400	—
2	6.8700	2.4239	—
3	5.3689	2.0776	—
4	4.5017	1.8463	—
5	3.9279	1.67685	2.5570
6	3.5156	1.5455	1.8469
7	3.2027	1.4397	1.6243
8	2.9555	1.3519	1.4851
9	2.7545	1.2776	1.3863
10	2.58705	1.2135	1.3120

equivalently,  $a, b_1 + b_2a + b_3a^2 + b_4a^3 = 0$ . This equation has a physical root,  $\alpha_{UV,4\ell} = \alpha_{UV,4\ell}/(4\pi)$ , as well as an unphysical pair of complex-conjugate values of  $a$ . We list values of  $\alpha_{UV,4\ell}$  in Table II as a function of  $N_f$ . As was the case with  $\alpha_{UV,3\ell}$ , in this  $\overline{\text{MS}}$  scheme,  $\alpha_{UV,4\ell}$  is a monotonically decreasing function of  $N_f$ . We find that when one goes from three loops to four loops, the UV zero decreases, i.e.,

$$\alpha_{UV,4\ell} < \alpha_{UV,3\ell} \quad \text{for fixed } N_f. \quad (9.9)$$

This decrease is substantial, roughly by a factor of 2.

### E. $\beta_{\alpha,5\ell}$

Recently, the five-loop coefficient has been calculated to be [40]

$$\begin{aligned} b_5 = N_f & \left[ \frac{4157}{6} + 128\zeta(3) \right. \\ & + \left( -\frac{7462}{9} - 992\zeta(3) + 2720\zeta(5) \right) N_f \\ & + \left( -\frac{21758}{81} + \frac{16000}{27}\zeta(3) - \frac{416}{3}\zeta(4) - \frac{1280}{3}\zeta(5) \right) N_f^2 \\ & \left. + \left( \frac{856}{243} + \frac{128}{27}\zeta(3) \right) N_f^3 \right]. \quad (9.10) \end{aligned}$$

Numerically,

$$\begin{aligned} b_5 = N_f & (846.6966 + 798.8919N_f - 148.7919N_f^2 \\ & + 9.22127N_f^3). \quad (9.11) \end{aligned}$$

This is positive for all non-negative  $N_f$ , both integral and real. The condition that  $\beta_{\alpha,5\ell}$  vanishes away from the origin is the quartic equation  $\sum_{\ell=1}^5 b_\ell \alpha^{\ell-1} = 0$ . We find that for  $N_f = 1, 2, 3, 4$ , this equation has no physical solutions. (It has two pairs of complex-conjugate solutions.) For some  $N_f \geq 5$ , we find that there are two positive real roots to this equation; the smaller of these is  $\alpha_{UV,5\ell}$ . We list the corresponding values of  $\alpha_{UV,5\ell}$  in Table II as a function of  $N_f$ . As is evident from this table, for values of  $N_f$  where the theory exhibits a physical value of  $\alpha_{UV,5\ell}$  in this  $\overline{\text{MS}}$  scheme, it is a monotonically decreasing function of  $N_f$ . We find that

$$\alpha_{UV,5\ell} > \alpha_{UV,4\ell} \quad \text{for fixed } N_f. \quad (9.12)$$

However, the slight increase in the value of the UV zero of  $\beta$  going from four-loop to five-loop order is smaller than the magnitude of the decrease going from three-loop to four-loop order, so that, for  $N_f$  values where  $\beta_{5\ell}$  has a UV zero,

$$\alpha_{UV,5\ell} < \alpha_{UV,3\ell} \quad \text{for fixed } N_f. \quad (9.13)$$

As is evident from Table II,  $\alpha_{UV,5\ell}$  is approximately half of the value of  $\alpha_{UV,3\ell}$ . These higher-loop results provide a quantitative measure of the effect of scheme dependence in the  $\beta$  function of the U(1) gauge theory. We have also

performed a corresponding analysis for an  $O(N)$ -symmetric  $\lambda\phi^4$  theory; the results will be reported elsewhere.

## X. CONCLUSIONS

Because terms at loop order  $\ell \geq 3$  in the  $\beta$  function of a gauge theory are scheme-dependent, it follows that one can carry out a scheme transformation to remove these terms at sufficiently small coupling. A basic question concerns the range of applicability of such a scheme transformation. It is particularly important to address this question when studying the IR zero that is present in the  $\beta$  function of an asymptotically free gauge theory for certain types of fermion content. In this paper, extending the study in [2], we have studied the properties of the scheme transformation  $S_{R,m}$  with  $m \geq 2$ , which renders the beta function coefficients  $b'_\ell = 0$  for  $3 \leq \ell \leq m + 1$ , at least for sufficiently small  $\alpha$ . We have calculated and presented expressions for the nonzero coefficients  $b'_\ell$  with  $\ell \geq m + 2$  resulting from the application of the  $S_{R,m}$  scheme transformation, up to the loop order  $\ell = 8$ . Since calculations with the scheme transformation  $S_{R,m}$  require a knowledge of the terms in the  $\beta$  function up to loop order  $\ell + 1$ ,  $S_{R,3}$  is the highest-order scheme transformation of this type that can be analyzed explicitly for a general non-Abelian gauge theory, using the beta function coefficients calculated up to four-loop order. We have carried out this analysis and have shown that the range of  $N_f$  values where the  $S_{R,3}$  scheme transformation is applicable is limited to  $N_f$  values in the upper part of the interval  $I$  where the two-loop  $\beta$  function has an IR zero at a correspondingly small value,  $\alpha_{IR,2\ell}$ . We have shown that this range of applicability is similar to that found for the  $S_{R,2}$  scheme transformation. For example, for an SU(3) gauge theory with  $N_f = 12$  fermions, neither  $S_{R,2}$  nor  $S_{R,3}$  can be used to study the IR fixed point because they produce unphysical effects. Our results elucidate the limitations on the use of scheme transformations to remove terms at loop order  $\ell \geq 3$  in the beta function of a gauge theory, a subject that does not seem to have received much attention in the literature. These results add to one's knowledge of the UV to IR evolution of an asymptotically free gauge theory, a fundamental topic in quantum field theory. We have also investigated scheme-dependent effects of higher-loop terms in the  $\beta$  function of a U(1) gauge theory.

## ACKNOWLEDGMENTS

This research was partially supported by the NSF Grant No. NSF-PHY-09-69739.

## APPENDIX A: EQUATIONS FOR THE $b'_\ell$ RESULTING FROM A GENERAL SCHEME TRANSFORMATION

The expressions for the  $b'_\ell$  in Eq. (3.3) for  $3 \leq \ell \leq 6$  are [2]

$$b'_3 = b_3 + k_1 b_2 + (k_1^2 - k_2) b_1, \quad (\text{A1})$$

$$b'_4 = b_4 + 2k_1 b_3 + k_1^2 b_2 + (-2k_1^3 + 4k_1 k_2 - 2k_3) b_1, \quad (\text{A2})$$

$$b'_5 = b_5 + 3k_1 b_4 + (2k_1^2 + k_2) b_3 + (-k_1^3 + 3k_1 k_2 - k_3) b_2 + (4k_1^4 - 11k_1^2 k_2 + 6k_1 k_3 + 4k_2^2 - 3k_4) b_1, \quad (\text{A3})$$

and

$$b'_6 = b_6 + 4k_1 b_5 + (4k_1^2 + 2k_2) b_4 + 4k_1 k_2 b_3 + (2k_1^4 - 6k_1^2 k_2 + 4k_1 k_3 + 3k_2^2 - 2k_4) b_2 + (-8k_1^5 + 28k_1^3 k_2 - 16k_1^2 k_3 - 20k_1 k_2^2 + 8k_1 k_4 + 12k_2 k_3 - 4k_5) b_1. \quad (\text{A4})$$

### APPENDIX B: HIGHER-ORDER COEFFICIENTS FOR $S_{R,m}$

In this appendix we list expressions for some higher-order coefficients  $k_s$  in the  $S_{R,m}$  scheme transformation. We calculate that

$$k_5 = \frac{b_6}{4b_1} - \frac{b_2 b_5}{6b_1^2} + \frac{2b_3 b_4}{b_1^2} + \frac{b_2^2 b_4}{12b_1^3} - \frac{b_2 b_3^2}{12b_1^3} \quad \text{for } S_{R,m} \quad (\text{B1})$$

with  $m \geq 5$ ,

$$k_6 = \frac{b_7}{5b_1} - \frac{3b_2 b_6}{20b_1^2} + \frac{8b_3 b_5}{5b_1^2} + \frac{11b_4^2}{20b_1^2} - \frac{4b_2 b_3 b_4}{5b_1^3} + \frac{b_2^2 b_5}{10b_1^3} + \frac{16b_3^3}{5b_1^3} + \frac{b_2^2 b_3^2}{20b_1^4} - \frac{b_2^3 b_4}{20b_1^4} \quad \text{for } S_{R,m} \quad \text{with } m \geq 6, \quad (\text{B2})$$

and

$$k_7 = \frac{b_8}{6b_1} - \frac{2b_2 b_7}{15b_1^2} + \frac{17b_3 b_6}{12b_1^2} + \frac{5b_4 b_5}{6b_1^2} + \frac{b_2^2 b_6}{10b_1^3} - \frac{9b_2 b_3 b_5}{10b_1^3} - \frac{49b_2 b_4^2}{120b_1^3} + \frac{19b_2^3 b_4}{3b_1^3} - \frac{b_2^3 b_5}{15b_1^4} - \frac{23b_2 b_3^3}{60b_1^4} + \frac{9b_2^2 b_3 b_4}{20b_1^4} + \frac{b_2^4 b_4}{30b_1^5} - \frac{b_2^3 b_3^2}{30b_1^5} \quad \text{for } S_{R,m} \quad \text{with } m \geq 7. \quad (\text{B3})$$

### APPENDIX C: PROPERTIES OF $S_{R,4}$ SCHEME TRANSFORMATION

In this appendix we give some relevant information on the next higher-order scheme transformation,  $S_{R,4}$ . The coefficients  $b'_\ell$  resulting from the application of the  $S_{R,4}$  scheme transformation are as follows, up to  $\ell = 8$  loop order:

$$b'_3 = b'_4 = b'_5 = 0, \quad (\text{C1})$$

$$b'_6 = b_6 - \frac{2b_2 b_5}{3b_1} + \frac{8b_3 b_4}{b_1} + \frac{b_2^2 b_4}{3b_1^2} - \frac{b_2 b_3^2}{3b_1^2}, \quad (\text{C2})$$

$$b'_7 = b_7 + \frac{8b_3 b_5}{b_1} + \frac{11b_4^2}{4b_1} + \frac{16b_3^3}{b_1^2} + \frac{2b_2 b_3 b_4}{b_1^2}, \quad (\text{C3})$$

$$b'_8 = b_8 + \frac{4b_3 b_6}{b_1} + \frac{5b_4 b_5}{b_1} - \frac{b_2 b_4^2}{4b_1^2} + \frac{2b_3^2 b_4}{b_1^2} + \frac{4b_2 b_3 b_5}{b_1^2} + \frac{12b_2 b_3^3}{b_1^3} - \frac{2b_2^2 b_3 b_4}{b_1^3}. \quad (\text{C4})$$

In general, after the  $S_{R,4}$  scheme transformation is applied, the resultant  $n$ -loop beta function,  $\beta'_{\alpha',n\ell}$ , has the form of Eq. (4.2) with  $m = 4$ .

When applied to an asymptotically free gauge theory with  $N_f \in I$ , so that there is an IR zero in  $\beta_{2\ell}$ , the transformation function  $f(a')$  evaluated at  $a'_{\text{IR},2\ell} = a_{\text{IR},2\ell} = -b_1/b_2$  is

$$f(a'_{\text{IR},2\ell}) = 1 + \frac{b_1 b_3}{b_2^2} - \frac{2b_1^2 b_4}{3b_2^3} + \frac{5b_1^2 b_3^2}{3b_2^4} + \frac{b_1^3 b_5}{3b_2^4}. \quad (\text{C5})$$

In order for the  $S_{R,4}$  scheme transformation to be acceptable, a necessary condition is  $C_1$ , that  $f(a') > 0$ , in particular, at  $a' = a'_{\text{IR},2\ell} = a_{\text{IR},2\ell}$ .

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However, for a given fermion mass  $m$ , as the reference scale  $\mu$  decreases below  $m$ , one would integrate these out of the low-energy effective theory applicable for  $\mu < m$ , so a massive fermion would not affect the UV to IR evolution significantly below its mass. Hence, to study the IR limit of this evolution, one may restrict to massless fermions.

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