# Generalized scheme transformations for the elimination of higher-loop terms in the beta function of a gauge theory

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We construct and study a generalized one-parameter class of scheme transformations, denoted  $S_{R,m,k_1}$ with  $m \ge 2$ , with the property that an  $S_{R,m,k_1}$  scheme transformation eliminates the  $\ell$ -loop terms in the beta function of a gauge theory from loop order  $\ell = 3$  to order  $\ell = m + 1$ , inclusive. These scheme transformations are applied to the higher-loop calculation of the infrared zero of the beta function of an asymptotically free gauge theory with multiple fermions. We show that scheme transformations in this generalized class satisfy a set of criteria for physical acceptability over a larger range of numbers of fermions than previously studied scheme transformations. We also present an interesting modification of a different type of scheme transformation that removes the three-loop term in the beta function.

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#### I. INTRODUCTION

A basic property of a gauge theory is the dependence of the gauge coupling  $g = g(\mu)$  on the Euclidean momentum scale,  $\mu$ , where it is measured. This is described by the beta function of the theory,  $\beta_q = dg/dt$  or, equivalently,  $\beta_{\alpha} = d\alpha/dt = [g/(2\pi)]\beta_{g}$ , where  $dt = d \ln \mu$  and  $\alpha(\mu) =$  $g(\mu)^2/(4\pi)$ . The 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 eliminates these terms and yields a beta function with only one- and two-loop terms [\[1\]](#page-12-0). In [\[2\]](#page-12-1) (with Ryttov), we constructed and studied explicit scheme transformations that remove terms at loop order  $\ell \geq 3$  from the beta function.

An important application of such scheme transformations is to the analysis of zero(s) of the beta function. The beta function of an asymptotically free non-Abelian gauge theory has an ultraviolet (UV) zero at  $\alpha = 0$ , which is an ultraviolet fixed point of the renormalization group. If the theory contains sufficiently many fermions, the (perturbatively calculated) beta function may also have an infrared (IR) zero at a point  $\alpha_{IR} > 0$ . Depending on how large  $\alpha_{IR}$  is, this zero is either an exact or approximate infrared fixed point (IRFP) of the renormalization group. Since the terms of loop order  $\ell \geq 3$  in the beta function are scheme dependent, so is the value of the IR zero when calculated to three-loop or higher-loop order. In order to understand the physical implications of this IR zero, it is necessary to assess the effect of scheme dependence on its value. A study of this dependence was carried out in [\[2\]](#page-12-1) using several scheme transformations. In [\[2\],](#page-12-1) we pointed out a set of criteria that a scheme transformation must satisfy in order to be physically acceptable, and showed that although it is straightforward for a scheme transformation to satisfy these criteria in the vicinity of a zero of the beta function at  $\alpha = 0$ , they are a significant restriction on the choice of an acceptable scheme transformation that can be applied at a generic infrared zero of the beta function. Examples of scheme transformations were given in [\[2\]](#page-12-1) that are acceptable for small  $\alpha$  but produce unphysical effects when applied at a generic IR zero of the beta function.

One type of procedure that would be natural for a quantitative study of scheme dependence of a zero of the beta function would be to construct and apply a scheme transformation that would remove successively higher and higher-loop terms in the beta function and, at each stage, determine how this removal shifted the position of the IR zero. Extending the results of [\[2\]](#page-12-1), in [\[3\]](#page-12-2) we defined a set of scheme transformations  $S_{R,m}$  with  $m \geq 2$  that remove the terms in the beta function at loop order  $l = 3$  to  $l = m + 1$ , inclusive, and determined the range of  $\alpha$  over which  $S_{R,2}$  and  $S_{R,3}$  can be applied to study the IR zero of the beta function of an asymptotically free gauge theory while satisfying the criteria to avoid introducing unphysical pathologies. For both  $S_{R,2}$  and  $S_{R,3}$ , it was shown that these ranges are rather limited, which, in turn, restricts one's ability to use these scheme transformations to study the scheme dependence of a zero of the beta function away from  $\alpha = 0$ .

In this paper, we present a generalized one-parameter class of scheme transformations, denoted  $S_{R,m,k_1}$  with  $m \geq 2$ , with the property that an  $S_{R,m,k_1}$  scheme transformation eliminates the  $\ell$ -loop terms in the beta function of a quantum field theory from loop order  $\ell = 3$  to order  $l = m + 1$ , inclusive. We give a detailed analysis of the application of this scheme transformation to the infrared zero of an asymptotically free gauge theory with gauge group  $G = SU(N_c)$  and  $N_f$  massless fermions in the fundamental representation, and we show that it satisfies the physical acceptability criteria specified in [\[2\]](#page-12-1) over a wider range of  $N_f$  and hence a wider range of values of an infrared zero,  $\alpha_{IR}$ , than those constructed and analyzed in [\[2,3\].](#page-12-1) We also investigate an interesting modification of the  $S_1$  scheme transformation presented in [\[2\]](#page-12-1).

This paper is organized as follows. In Sec. [II,](#page-1-0) we recall some basic information and notation that will be needed for our analysis. In Sec. [III,](#page-3-0) we define the scheme transformation  $S_{R,m,k_1}$ . We display explicit expressions for the resultant coefficients in the beta function resulting from the application of the  $S_{R,m,k_1}$  transformation in Sec. [IV.](#page-4-0) In Secs. [V](#page-5-0) and [VI,](#page-6-0) we present specific results on the application of the respective scheme transformations  $S_{R,2,k_1}$  and  $S_{R,3,k_1}$  to an IR zero in the beta function of an  $SU(N_c)$  gauge theory. In Sec. [VII,](#page-7-0) we give further results on the application of these scheme transformations in the limit  $N_c \rightarrow \infty$  and  $N_f \rightarrow \infty$  with the ratio  $N_f/N_c$ fixed. In Sec. [VIII,](#page-10-0) we discuss a modification of a different type of scheme transformation, namely, the  $S_1$  transformation of [\[2\]](#page-12-1). We present our conclusions in Sec. [IX](#page-10-1). Some additional results are included in the appendixes.

#### II. BASICS

<span id="page-1-0"></span>In this section, we recall some basic formalism and notation that will be used in our analysis. The scheme transformation  $S_{R,m,k_1}$  that we construct and study can be applied to any gauge theory, vectorial or chiral, and non-Abelian or Abelian. Indeed, this transformation can also be applied to a quantum field theory that does not involve gauge fields, with an appropriate replacement of  $q$  by the relevant interaction coupling. Here, we will focus on the application to a vectorial non-Abelian gauge theory with gauge group G and a set of  $N_f$  massless fermions transforming according to a representation  $R$  of  $G$ . Since these theories are vectorial, the gauge invariance would allow nonzero fermion masses. However, in studying the evolution of the gauge coupling as a function of the scale  $\mu$ , as this scale decreases below the value of a given fermion mass, one would construct a low-energy effective field theory by integrating this fermion out, so this massive fermion would not affect the evolution of the coupling for scales below its mass. Hence, our assumption of massless fermions does not entail a loss of generality.

It will be convenient to define the quantity

$$
a(\mu) \equiv \frac{\alpha(\mu)}{4\pi} = \frac{g(\mu)^2}{16\pi^2}.
$$
 (2.1)

<span id="page-1-1"></span>(The argument  $\mu$  will often be suppressed in the notation.) The  $\beta_{\alpha}$  function has the power-series expansion

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

where  $\ell$  labels the loop order,  $\bar{b}_{\ell} = b_{\ell}/(4\pi)^{\ell}$ , and we have extracted a minus sign so that the one-loop coefficient  $b_1$  is positive if the theory is asymptotically free. The  $n$ -loop (*nl*) β function, denoted  $\beta_{\alpha,n\ell}$ , is obtained from Eq. [\(2.2\)](#page-1-1) by replacing the upper limit on the  $\ell$ -loop summation by n instead of ∞. The (scheme-independent) one-loop and twoloop coefficients  $b_1$  and  $b_2$  were calculated in [\[4\]](#page-12-3) and [\[5,6\]](#page-12-4), respectively, and are listed for reference in Appendix [A](#page-10-2). As mentioned above, the  $b_\ell$  with  $\ell \geq 3$  are scheme dependent [\[7,8\].](#page-13-0) For a non-Abelian gauge theory,  $b_3$  and  $b_4$  were calculated in [\[9\]](#page-13-1) and [\[10\]](#page-13-2) in the modified minimal subtraction scheme [\[11\].](#page-13-3) The property of asymptotic freedom, i.e.,  $b_1 > 0$ , requires that  $N_f < N_{f,b1z}$ , where  $N_{f,b1z} =$  $11C_A/(4T_f)$  [\[12\]](#page-13-4). We assume that this condition is satisfied.

If an asymptotically free gauge theory has sufficiently many massless fermions, the beta function can exhibit an IR zero at a certain value, denoted generically as  $\alpha_{IR}$  [\[5,13\]](#page-12-4). As is evident from Eq. [\(A2\)](#page-11-0), for small  $N_f$ ,  $b_2$  is positive, but it decreases with increasing  $N_f$  and passes through zero to negative values as  $N_f$  increases through the value

$$
N_{f,b2z} = \frac{34C_A^2}{4(5C_A + 3C_f)T_f}.
$$
 (2.3)

<span id="page-1-3"></span>Since  $N_{f,b2z} < N_{f,b1z}$ , there is always an interval *I*, defined by

$$
I: N_{f,b2z} < N_f < N_{f,b1z}, \tag{2.4}
$$

<span id="page-1-2"></span>in which the two-loop beta function,  $\beta_{\alpha,2\ell}$ , has an IR zero. For  $N_f \in I$ , this zero of  $\beta_{\alpha,2\ell}$  occurs at the (schemeindependent) value

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

Henceforth, for definiteness, we focus on the case where the gauge group is  $G = SU(N_c)$  and the  $N_f$  fermions transform according to the fundamental representation.

If the IR zero of the beta function occurs at a small value of the gauge coupling, then this is an exact IRFP of the renormalization group. With decreasing  $N_f$ ,  $\alpha_{\text{IR}}$  increases, eventually to a value at which the gauge interaction is strong enough to trigger the formation of bilinear fermion condensates with associated spontaneously chiral symmetry breaking  $(S \chi SB)$ . As a consequence of this, the fermions gain dynamical masses of order the  $S\chi SB$  scale, denoted Λ. In the low-energy effective field theory applicable at scales  $\mu < \Lambda$ , these fermions are integrated out, the beta function changes to one with  $N_f = 0$ , and the resultant low-energy theory does not have an IR zero in its (perturbative) beta function. Thus, in this case, the initial zero is only an approximate, rather than exact, fixed point of the renormalization group. The value of  $N_f$  that separates these two regimes of infrared behavior is denoted  $N_{f,cr}$ . If the beta function of a theory has an IR zero that is only slightly greater than the minimum value for fermion condensation, then the UV to IR evolution exhibits slowly running, quasi-scale-invariant behavior over a substantial interval of scales  $\mu$ . This behavior, and the resultant approximate Nambu-Goldstone boson (the dilaton) that results from the spontaneous breaking of scale invariance by the bilinear fermion condensate, might be relevant for physics beyond the Standard Model [\[14\]](#page-13-5).

Since  $N_{f,cr}$  corresponds to a value  $\alpha \sim O(1)$  for the exact or approximate infrared zero of the beta function, one is motivated to calculate this value to higher-loop order [\[15\]](#page-13-6). This was done in [\[16,17\]](#page-13-7) for this zero of the beta function and for the corresponding value of the anomalous dimension of the fermion bilinear for a general gauge group and fermion representation. Additional higher-loop results on structural properties of the beta function were calculated in [\[18](#page-13-8)–20]. In turn, this motivated the study of the scheme dependence of the IR zero in beta in [\[2,3\]](#page-12-1) (some related work is in [\[21](#page-13-9)–25]).

<span id="page-2-4"></span>A scheme transformation can be expressed as a mapping between  $\alpha$  and  $\alpha'$ , or equivalently,  $\alpha$  and  $\alpha'$ , which we write as

$$
a = a' f(a'), \tag{2.6}
$$

where  $f(a')$  is the scheme transformation function. The properties of the theory must remain unchanged under a scheme transformation in the limit in which the gauge coupling vanishes and the theory becomes free, which implies the condition that  $f(0) = 1$ . We will use a function  $f(a')$  that is analytic about  $a = a' = 0$  and hence has the power-series expansion

<span id="page-2-3"></span>
$$
f(a') = 1 + \sum_{s=1}^{s_{\text{max}}} k_s(a')^s = 1 + \sum_{s=1}^{s_{\text{max}}} \bar{k}_s(a')^s, \qquad (2.7)
$$

where the  $k_s$  are constants,  $\bar{k}_s = k_s/(4\pi)^s$ , and  $s_{\text{max}}$  may be finite or infinite. The Jacobian of this transformation is  $J = da/da' = da/da'$ , with the expansion

$$
J = 1 + \sum_{s=1}^{s_{\text{max}}} (s+1)k_s(a')^s = 1 + \sum_{s=1}^{s_{\text{max}}} (s+1)\bar{k}_s(a')^s.
$$
\n(2.8)

<span id="page-2-2"></span>This Jacobian thus has the value  $J = 1$  at  $a = a' = 0$ . After the scheme transformation is applied, the beta function in the resultant scheme is

$$
\beta_{\alpha'} \equiv \frac{d\alpha'}{dt} = \frac{d\alpha'}{d\alpha} \frac{d\alpha}{dt} = J^{-1}\beta_{\alpha}.
$$
 (2.9)

<span id="page-2-0"></span>This has the expansion

$$
\beta_{\alpha'} = -2\alpha' \sum_{\ell=1}^{\infty} b_{\ell}'(a')^{\ell} = -2\alpha' \sum_{\ell=1}^{\infty} \bar{b}_{\ell}'(\alpha')^{\ell}, \qquad (2.10)
$$

with a new set of coefficients  $b'_\ell$  [where  $\bar{b}'_\ell = b'_\ell/(4\pi)^\ell$ ]. One then solves for the  $b'_\ell$  as functions of the  $b_\ell$  and  $k_s$ . This gives  $b'_1 = b_1$  and  $b'_2 = b_2$  and the new results for  $b'_e$ at higher-loop order  $\ell$  that were presented in [\[2\]](#page-12-1). For the reader's convenience, we list some of these results in Appendix [B.](#page-11-1)

The *n*-loop beta function in the transformed scheme,  $\beta_{\alpha',n\ell}$ , is given by Eq. [\(2.10\)](#page-2-0) with the upper limit on the  $\ell$ summation equal to *n* rather than  $\infty$ . It will be useful to extract the quadratic prefactors and define

$$
\beta_{\alpha,n\ell,r} \equiv -\frac{\beta_{\alpha,n\ell}}{2\alpha^2} = \sum_{\ell=1}^n \bar{b}_{\ell}\alpha^{\ell-1} = \frac{1}{4\pi} \sum_{\ell=1}^n b_{\ell}\alpha^{\ell-1} \qquad (2.11)
$$

and similarly with  $\beta_{\alpha',n\ell,r}$ , with the replacements  $\alpha \to \alpha'$ ,  $b_{\ell} \rightarrow b'_{\ell}$ , and  $\bar{b}_{\ell} \rightarrow \bar{b}'_{\ell}$ . Since  $b'_1 = b_1$  and  $b'_2 = b_2$ , it follows that

$$
\beta_{\alpha',2\ell} = \beta_{\alpha,2\ell}.\tag{2.12}
$$

<span id="page-2-1"></span>Consequently, if  $\beta_{\alpha,2\ell}$  has a (UV or IR) zero at  $\alpha_{z,2\ell}$ , then  $\beta_{\alpha',2\ell}$  also has a (UV or IR) zero, and at the same value in the transformed variable,

$$
\alpha'_{z,2\ell} = \alpha_{z,2\ell}.\tag{2.13}
$$

We will use this property below for asymptotically free gauge theories, where this is an IR zero, so the equality [\(2.13\)](#page-2-1) reads [\[26\]](#page-13-10)

$$
\alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell} = -\frac{4\pi b_1}{b_2}.
$$
 (2.14)

We recall the set of conditions that a scheme transformation must satisfy in order to be physically acceptable [\[2,3\].](#page-12-1) The first of these, which we label as condition  $C_1$ , is that the scheme transformation must transform a real positive  $\alpha$  to a real positive  $\alpha'$ , since a function mapping  $\alpha > 0$  to  $\alpha' = 0$  would be singular, and a function mapping  $\alpha > 0$  to a negative or complex  $\alpha'$  would violate unitarity. The second condition,  $C_2$ , is that the scheme transformation should transform a small or moderate value of  $\alpha$  to a similarly small or moderate value of  $\alpha'$ , so a perturbative analysis remains valid. The third condition,  $C_3$ , is that the Jacobian J must be nonzero to avoid a singular trans-formation [\(2.9\)](#page-2-2). Since  $J = 1$  at  $\alpha = \alpha' = 0$  and J is a continuous function, condition  $C_3$  implies that  $J > 0$ . The zero of  $\beta$  is a scheme-independent property, and hence, as the fourth condition,  $C_4$ , a scheme transformation should be such that  $\beta_{\alpha}$  has a zero if and only if  $\beta_{\alpha'}$  has a zero. The conditions apply for both a scheme transformation and its inverse.

These conditions can easily be satisfied by scheme transformations applied in the vicinity of  $\alpha = 0$ , such as those used to optimize the convergence of perturbative calculations in quantum chromodynamics [\[27\]](#page-13-11), but they are a significant constraint on a scheme transformation applied in the vicinity of a (UV or IR) zero of the beta function for  $\alpha \lesssim O(1)$ . Underlying this analysis of scheme transformations is, of course, the assumption that one is studying the theory for values of the coupling  $\alpha$  that are sufficiently small such that perturbative calculations are justified. Clearly, if the value of  $\alpha$  at the zero of the beta function is too large, then one cannot use perturbative calculational methods reliably. From the expression for the zero of the beta function,  $\alpha_{IR,2\ell}$  in Eq. [\(2.5\),](#page-1-2) it is evident that this gets large as  $N_f$  decreases toward the lower end of the interval I at  $N_{f,b2z}$  and  $b_2$  approaches zero. Hence, one cannot reliably use perturbative methods to study the evolution of the coupling near this lower end of the interval I. Since scheme transformations are carried out in the context of perturbative calculations, it follows that one could optionally relax the requirement that a scheme transformation must satisfy all of the conditions  $C_1$ - $C_4$  at the lower end of this interval I.

# <span id="page-3-0"></span>III. GENERAL CLASS OF SCHEME TRANSFORMATIONS  $S_{R,m,k_1}$  AND  $S_{R,\infty,k_1}$

In this section, we present a new scheme transformation  $S_{R,m,k_1}$ , with  $m \geq 2$  and  $s_{\text{max}} = m$ , that removes the terms in the beta function  $\beta_{\alpha'}$  from loop order  $\ell = 3$  to order  $l = m + 1$ , inclusive. In our notation, we have specifically included the value of  $k_1$ , since a choice for  $k_1$  determines the  $k<sub>s</sub>$  for  $s \ge 2$ . Applying the scheme transformation  $S_{R,m,k_1}$  to an initial scheme, it follows that

<span id="page-3-1"></span>
$$
S_{R,m,k_1} \Rightarrow b'_{\ell} = 0 \text{ for } \ell = 3, ..., m+1. \tag{3.1}
$$

<span id="page-3-2"></span>Thus,  $S_{R,m,k_1}$  yields

$$
\beta_{\alpha',n\ell} = -8\pi (a')^2 \bigg[ b_1 + b_2 a' + \sum_{\ell=m+2}^n b'_\ell (a')^{\ell-1} \bigg], \quad (3.2)
$$

<span id="page-3-5"></span>and similarly for the expansion in powers of  $\alpha$ , with  $b'_{\ell}$ replaced by  $\bar{b}'_e$ . From Eq. [\(3.1\),](#page-3-1) it follows that a zero of the *n*-loop beta function  $\beta_{\alpha', m\ell}$  is at the same value as the (scheme-independent) value  $\alpha_{IR,2\ell}$  for *n* up to and including  $n = m + 1$ , i.e.,

$$
S_{R,m} \Rightarrow \alpha'_{\text{IR},n\ell} = \alpha_{\text{IR},2\ell} \quad \text{for } n = 3, ..., m + 1. \tag{3.3}
$$

The construction of this scheme makes use of the property that the resultant 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. The choice of  $k_1$ , together with the values of the  $b_{\ell}$ , thus uniquely determines the  $k_s$  for  $s \geq 2$ . The simplest choice is  $k_1 = 0$ , and this was studied in detail in [\[2,3\].](#page-12-1) This special case is indicated with the notation

$$
S_{R,m,k_1=0} \equiv S_{R,m}.\tag{3.4}
$$

<span id="page-3-3"></span>Here we present, as new results, the general formulas for the  $k_s$  in the  $S_{R,m,k_1}$  scheme with nonzero  $k_1$ . The first step is to use Eq. [\(B1\)](#page-11-2) and solve the equation  $b'_3 = 0$  for  $k_2$ . This yields the result

$$
k_2 = \frac{b_3}{b_1} + \frac{b_2}{b_1}k_1 + k_1^2 \quad \text{for } S_{R,m,k_1} \quad \text{with} \quad m \ge 2. \tag{3.5}
$$

<span id="page-3-4"></span>This suffices for  $S_{R,2,k_1}$ . To obtain  $S_{R,m,k_1}$  with  $m \geq 3$ , removing the  $l = 3, 4$  terms in  $\beta_{\alpha}$ , we need to compute  $k_3$ . For this purpose, we substitute the values of  $k_1$  and  $k_2$  into Eq. [\(B2\)](#page-11-3) and solve the equation  $b'_4 = 0$  for  $k_3$ . This gives

$$
k_3 = \frac{b_4}{2b_1} + \frac{3b_3}{b_1}k_1 + \frac{5b_2}{2b_1}k_1^2 + k_1^3 \quad \text{for } S_{R,m,k_1} \quad \text{with}
$$
  

$$
m \ge 3. \tag{3.6}
$$

Next, to obtain  $k_4$ , as needed for  $S_{R,m,k_1}$  with  $m \geq 4$ , we substitute the  $k_s$  with  $s = 1, 2, 3$  into Eq. [\(B3\)](#page-11-4) and solve the equation  $b'_5 = 0$  for  $k_4$ . This yields

$$
k_4 = \frac{b_5}{3b_1} - \frac{b_2b_4}{6b_1^2} + \frac{5b_3^2}{3b_1^2} + \left(\frac{2b_4}{b_1} + \frac{3b_2b_3}{b_1^2}\right)k_1
$$
  
+ 
$$
\left(\frac{6b_3}{b_1} + \frac{3b_2^2}{2b_1^2}\right)k_1^2 + \left(\frac{13b_2}{3b_1}\right)k_1^3 + k_1^4
$$
  
for  $S_{R,m,k_1}$  with  $m \ge 4$ . (3.7)

We continue this procedure iteratively to calculate  $S_{R,m,k_1}$ for higher m. Thus, having computed the  $k<sub>s</sub>$  up to order  $s = m - 1$  inclusive, we compute  $k_m$  by substituting these  $k_s$  with  $1 \le s \le m-1$  into our expression for  $b'_{m+1}$  and solving the equation  $b'_{m+1} = 0$  for  $k_m$ . For a given  $k_1$ , this yields a unique solution for  $k_m$  because, as noted above, the equation  $b'_{m+1} = 0$  with  $m + 1 \ge 3$  is a linear equation in  $k_m$ . Specifically, in the expression for  $b'_{m+1}$  with  $m + 1 \geq 3$ , the variable  $k_m$  occurs only in the term  $-(m-1)k_m b_1$ . We list the  $k_s$  for  $s = 5$  and  $s = 6$  in Appendix [C.](#page-11-5) These expressions become progressively lengthier as s increases, but our method for calculating them as solutions to respective linear equations is systematic for any s. As is evident, the choice  $k_1 = 0$  greatly simplifies these expressions for the  $k<sub>s</sub>$  with  $s \ge 2$  and hence also the transformation function  $f(a')$ . However, as was shown in [\[2,3\],](#page-12-1) with this choice of  $k_1 = 0$ , the scheme transformation  $S_{R,m}$  leads to violations of one or more of the requisite conditions  $C_1$ - $C_4$  when applied to the IR zero of the beta function in an asymptotically free non-Abelian gauge theory with fermions for a substantial range of  $N_f \in I$ . With our generalization, taking advantage of the extra parameter  $k_1$  on which the scheme transformation  $S_{R,m,k_1}$  depends, we obtain a significantly enlarged range of applicability of this scheme transformation at an IR zero of the beta function.

Because the scheme transformation  $S_{R,m,k_1}$  involves coefficients  $k_s$  with  $s = 2, ..., m$ , the construction of this scheme transformation requires a knowledge of the  $b_{\ell}$  in this initial scheme up to the loop order  $l = m + 1$ . Since  $s_{\text{max}} = m$  for  $S_{R,m,k_1}$ , it follows that  $k_s = 0$  for  $S_{R,m,k_1}$  with  $s > m$ . For a given  $k_1$ , using the  $k_s$  with  $s = 2, ..., m$  as calculated via the procedure above, we compute the  $f(a')$ function for the  $S_{R,m,k_1}$  scheme transformation:

$$
f(a')_{S_{R,m,k_1}} = 1 + \sum_{s=1}^{m} k_s(a')^s = 1 + \sum_{s=1}^{m} \bar{k}_s(a')^s. \quad (3.8)
$$

Applying this to an initial scheme, we obtain  $b'_e = 0$  for  $l = 3, ..., m + 1$ , as in [\(3.1\)](#page-3-1)–[\(3.2\)](#page-3-2).

The generalized scheme transformation  $S_{R,m,k_1}$  satisfies the same scaling properties that we derived in [\[2\]](#page-12-1) for the case  $k_1 = 0$ , i.e., the  $S_{R,m}$  transformation. Thus, the coefficient  $k_s$  depends on the  $b_\ell$  with  $\ell = 1, ..., s + 1$ via the ratios  $b_{\ell}/b_1$  for  $\ell = 2, ..., s + 1$ , and consequently, these  $k_s$  are invariant under the rescaling  $b_\ell \rightarrow \lambda b_\ell$ , where  $\lambda \in \mathbb{R}$ . It follows that  $S_{R,m,k_1}$  is invariant under the rescaling  $b_{\ell} \rightarrow \lambda b_{\ell}$ . As was true of  $S_{R,m}$ , since  $S_{R,m,k_1}$  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 [\[9,10\]](#page-13-1), the highest order for which we can calculate and apply the  $S_{R,m,k_1}$  scheme transformation is  $m = 3$ .

The application of the transformation  $S_{R,m,k_1}$  to an arbitrary initial scheme yields a  $\beta_{\alpha'}$  function with  $b'_{\ell} = 0$ for  $l = 3, ..., m + 1$ , as expressed in Eqs. [\(3.1\)](#page-3-1)–[\(3.2\)](#page-3-2), so in the new scheme, the IR zero of the  $n$ -loop beta function  $\beta_{\alpha',m\ell}$  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.,  $\alpha'_{\text{IR},n\ell} = \alpha_{\text{IR},2\ell}$  for  $n = 3,...,m+1$ .

We define  $S_{R,\infty,k_1} = \lim_{m \to \infty} S_{R,m,k_1}$ . Assuming that  $S_{R,\infty,k_1}$  meets the conditions to be physically acceptable, it takes an arbitrary initial scheme to a scheme with  $b'_e = 0$ for all  $l \geq 3$ , so that  $\beta_{\alpha'} = -8\pi (a')^2 (b_1 + b_2 a') =$  $-2(\alpha')^2(\bar{b}_1+\bar{b}_2\alpha').$ 

# <span id="page-4-0"></span>IV. COEFFICIENTS  $b'_\ell$  RESULTING FROM  $S_{R,m,k_1}$ SCHEME TRANSFORMATION

#### A. General properties

We note some general structural properties of the coefficients  $b'_{\ell}$  for  $S_{R,m,k_1}$ . First, in the expression for  $b'_{\ell}$ , the sum of the subscripts of the  $b_{\ell}$  factors in the numerator of each term minus the power of  $b_1$  in the denominator (if present) plus the power of  $k_1$  which multiplies this term is equal to  $\ell$ . For example, in the expression for the coefficient  $b'_5$  resulting from the application of the  $S_{R,2,k_1}$ scheme transformation in Eq. [\(4.3\)](#page-4-1) below, in the term  $(12b_2b_3/b_1)k_1$ , this sum is  $2 + 3 - 1 + 1 = 5$ , and so forth

for the other terms in Eq. [\(4.3\)](#page-4-1) and the other  $b'_e$ . The (nonzero) coefficient  $b'_{\ell}$  resulting from the scheme trans-formation [\(2.7\)](#page-2-3) is, in general, a polynomial in the  $k<sub>s</sub>$  for  $s = 1, ..., \ell - 1$ , and the term in  $b'_{\ell}$  of highest degree in  $k_1$ is proportional to  $k_1^{\ell-1}$ . It follows, in particular, that the term in the nonzero coefficient  $b'_\ell$  resulting from the  $S_{R,m,k_1}$ scheme transformation (and hence with  $l \ge m + 2$ ) is a polynomial in  $k_1$  with the property that its highest-degree term has at most degree  $\ell - 1$ . Actually, in several cases, the coefficient of the  $k_1^{\ell-1}$  term in  $b'_\ell$  vanishes, so the highest-degree term is proportional to  $k_1^{\ell-2}$ . This happens, for example, for coefficient  $b'_6$  resulting from the  $S_{R,2,k_1}$ scheme transformation and for the coefficients  $b'_{\ell}$  with  $l = 7, 8$  resulting from the  $S_{R,3,k_1}$  scheme transformation.

# **B.**  $S_{R,2,k_1}$

<span id="page-4-2"></span>Here we give the coefficients  $b'_\ell$  resulting from applying the scheme transformation  $S_{R,2,k_1}$  to an initial scheme. From the expressions for the  $k_s$  in the  $S_{R,2,k_1}$  transformation, we obtain the following results for  $s = 3, 4, 5$ :

$$
b'_3 = 0, \t\t(4.1)
$$

$$
b'_4 = b_4 + 6b_3k_1 + 5b_2k_1^2 + 2b_1k_1^3, \tag{4.2}
$$

<span id="page-4-1"></span>and

$$
b'_5 = b_5 + \frac{5b_3^2}{b_1} + \left(3b_4 + \frac{12b_2b_3}{b_1}\right)k_1 + \frac{7b_2^2}{b_1}k_1^2
$$
  
-  $b_2k_1^3 - 3b_1k_1^4$ . (4.3)

The expressions for  $b'_{\ell}$  for higher s are more lengthy and are given in Appendix [D.](#page-11-6) The expression for the  $n$ -loop beta function  $\beta_{\alpha',n\ell}$  resulting from the application of the  $S_{R,2,k_1}$  transformation is given by the  $m = 2$  special case of Eq. [\(3.2\)](#page-3-2).

## C.  $S_{R,3,k_1}$

We next present the coefficients  $b'_{\ell}$  resulting from applying the scheme transformation  $S_{R,3,k_1}$  to an initial scheme. From the expressions for the  $k_s$  in the  $S_{R,3,k_1}$  transformation, we obtain the following results for  $s = 3, 4, 5$ :

<span id="page-4-3"></span>and

$$
b'_5 = b_5 + \frac{5b_3^2}{b_1} - \frac{b_2b_4}{2b_1} + \left(6b_4 + \frac{9b_2b_3}{b_1}\right)k_1
$$
  
+ 
$$
\left(18b_3 + \frac{9b_2^2}{2b_1}\right)k_1^2 + 13b_2k_1^3 + 3b_1k_1^4.
$$
 (4.5)

 $b'_3 = 0, \qquad b'_4 = 0,$  (4.4)

We list the expressions for  $b'_{\ell}$  with higher s in Appendix [E](#page-12-5). The expression for the *n*-loop beta function  $\beta_{\alpha',n\ell}$  following from the application of the  $S_{R,3,k_1}$  transformation is given by the  $m = 3$  special case of Eq. [\(3.2\).](#page-3-2)

In a similar manner, one can calculate the coefficients for the  $S_{R,m,k_1}$  scheme transformations with  $m \geq 4$ . However, to actually apply these scheme transformations to a given theory requires knowledge of the  $b_{\ell}$  coefficients up to loop order  $\ell = m + 1$ , i.e.,  $\ell \geq 5$  for  $m \geq 4$ . Since our primary application will be to non-Abelian gauge theories, and since the  $b_{\ell}$  have only been calculated up to loop order  $\ell = 4$ , we thus limit ourselves to studying the application of the scheme transformations  $S_{R,m,k_1}$  with  $m = 2$ and  $m = 3$ .

## <span id="page-5-0"></span>V. APPLICATION OF THE  $S_{R,2,K_1}$  SCHEME TRANSFORMATION

In this section and the next, we discuss the application of the  $S_{R,m,k_1}$  scheme transformations. These transformations can be applied to the beta function of any gauge theory, non-Abelian or Abelian, asymptotically free or infraredfree. As mentioned in the Introduction, we will focus here on the application to the study of an infrared zero in the beta function of an asymptotically free vectorial gauge non-Abelian gauge theory with gauge group G and  $N_f$  massless Dirac fermions in a representation  $R$  of  $G$ . Note that the two-loop beta function for an Abelian U(1) gauge theory does not have a zero away from the origin (which would be a UV zero), since  $b_1$  and  $b_2$  have the same sign (see, e.g., [\[25\]](#page-13-12) and references therein).

In previous work  $[2,3]$ , it was shown that the special case of the  $S_{R,2,k_1}$  scheme transformation with  $k_1 = 0$ , denoted  $S_{R,2} \equiv S_2$ , cannot be applied to a generic IR zero of an asymptotically free  $SU(N_c)$  gauge theory because for a given  $N_c$  it fails to satisfy the requisite conditions to be physically acceptable for a substantial part of the interval I in Eq. [\(2.4\).](#page-1-3) Here we show that one can pick the parameter  $k_1$  in our generalized one-parameter scheme transformation  $S_{R,2,k_1}$  so as to avoid the pathologies encountered with the  $S_{R,2} \equiv S_{R,2,k_1=0}$  transformation.

The  $f(a')$  function for the  $S_{R,2,k_1}$  scheme transformation is given by

$$
S_{R,2,k_1}: f(a') = 1 + k_1 a' + \left(\frac{b_3}{b_1} + \frac{b_2}{b_1}k_1 + k_1^2\right)(a')^2
$$
  
= 1 +  $\bar{k}_1 a' + \left(\frac{\bar{b}_3}{\bar{b}_1} + \frac{\bar{b}_2}{\bar{b}_1}\bar{k}_1 + \bar{k}_1^2\right)(a')^2,$  (5.1)

and hence the Jacobian is

$$
S_{R,2,k_1}: J = 1 + 2k_1a' + 3\left(\frac{b_3}{b_1} + \frac{b_2}{b_1}k_1 + k_1^2\right)(a')^2
$$
  
= 1 + 2\bar{k}\_1a' + 3\left(\frac{\bar{b}\_3}{\bar{b}\_1} + \frac{\bar{b}\_2}{\bar{b}\_1}\bar{k}\_1 + \bar{k}\_1^2\right)(a')^2. (5.2)

Now, assume that  $N_f \in I$ , so that there is an IR zero in the two-loop beta function,  $\beta_{2\ell}$ , as given in Eq. [\(2.5\).](#page-1-2) Since the existence of an IR zero in beta is a scheme-independent property, one may impose the condition on an acceptable scheme that it should maintain this property at higherloop level. Because the three-loop expression for the zero of  $\beta_{\alpha}$  away from the origin involves the square root  $\sqrt{b_2^2 - 4b_1b_3}$ , and because  $b_2 \rightarrow 0$  at the smaller-N<sub>f</sub> end of the interval I, this condition generically implies that the scheme should be such that  $b_3 < 0$  for  $N_f \in I$  [\[19\]](#page-13-13). In particular, this condition is satisfied in the  $\overline{\text{MS}}$  scheme [\[16\]](#page-13-7). We shall impose this condition in the following. From our discussion above, it follows that

$$
\alpha'_{\text{IR},3\ell} = \alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell},\tag{5.3}
$$

provided that the  $S_{R,2,k_1}$  transformation is acceptable.

As in our earlier works [\[2,3\],](#page-12-1) the scheme dependence of the theory in the vicinity of the IR zero of the beta function is of particular interest, so we focus on this. The requirement that the  $S_{R,2,k}$  scheme transformation should obey condition  $C_1$ , mapping  $a' > 0$  to  $a > 0$ , is that  $f(a') > 0$ . This inequality must be satisfied, in particular, at  $a'_{IR,2l}$  $a_{\text{IR},2\ell} = -b_1/b_2$ . Evaluating  $f(a')$  at this value, we obtain

<span id="page-5-1"></span>
$$
S_{R,2,k1}: f(a'_{\text{IR},2\ell}) = 1 + \frac{b_1 b_3}{b_2^2} + \frac{b_1^2}{b_2^2} k_1^2,
$$
 (5.4)

<span id="page-5-2"></span>and hence the inequality

$$
1 + \frac{b_1 b_3}{b_2^2} + \frac{b_1^2}{b_2^2} k_1^2 > 0.
$$
 (5.5)

<span id="page-5-4"></span>[Note that the terms linear in  $k_1$  in [\(5.4\)](#page-5-1) and [\(5.5\)](#page-5-2) happen to vanish here and also below in Eq. [\(7.14\)](#page-8-0).] Because the coefficient of  $k_1^2$  is positive, this inequality can always be satisfied by using a value of  $k_1^2$  that satisfies the inequality

$$
k_1^2 > (k_1^2)_{\min},\tag{5.6}
$$

<span id="page-5-3"></span>where

$$
(k_1^2)_{\min} = -\frac{(b_2^2 + b_1 b_3)}{b_1^2} = \frac{-b_2^2 + b_1 |b_3|}{b_1^2}.
$$
 (5.7)

In Eq. [\(5.7\),](#page-5-3) we have used the property that  $b_3 < 0$  for  $N_f \in I$ . By a continuity argument, if  $f(a') > 0$  at  $a' = a'_{\text{IR},2\ell}$ , then this is also true in a neighborhood of this point on the real  $a'$  axis. Equation [\(5.7\)](#page-5-3) is a nontrivial condition if  $b_3$  is sufficiently negative that  $|b_3| > b_2^2/b_1$ . As was shown in  $[2,3]$ , such a subinterval in *I* does exist if one uses the  $\overline{\text{MS}}$  scheme as the initial scheme. Indeed, this is the reason why  $S_{R,2} = S_{R,2,0}$  violates condition  $C_1$ .

Condition  $C_3$  is that  $J > 0$ , in particular, at  $a'_{IR,2\ell} =$  $a_{\text{IR},2\ell} = -b_1/b_2$ . Evaluating J at this value, we obtain

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$$
S_{R,2,k1}: J = 1 + \frac{3b_1b_3}{b_2^2} + \frac{b_1}{b_2}k_1 + \frac{3b_1^2}{b_2^2}k_1^2.
$$
 (5.8)

<span id="page-6-1"></span>Then  $C_3$  is the inequality

$$
1 + \frac{3b_1b_3}{b_2^2} + \frac{b_1}{b_2}k_1 + \frac{3b_1^2}{b_2^2}k_1^2 > 0.
$$
 (5.9)

If  $k_1$  were zero, then, since  $b_3 < 0$ , this condition would be violated for  $|b_3| > b_2^2/(3b_1)$ . For a given  $N_c$ , as  $N_f \in I$ increases and  $b_3$  increases in magnitude through negative values, J goes negative before  $f(a')$  does, since  $|b_3|$ exceeds  $b_2^2/(3b_1)$  before it exceeds  $b_2^2/b_1$ . Taking into account that  $b_2 < 0$  and  $b_3 < 0$  in *I*, the inequality [\(5.9\)](#page-6-1) is satisfied if

<span id="page-6-2"></span>
$$
k_1 > \frac{1}{6b_1} \left( |b_2| + \sqrt{-11b_2^2 + 36b_1|b_3|} \right) \tag{5.10}
$$

<span id="page-6-3"></span>or

$$
k_1 < \frac{1}{6b_1} \left( |b_2| - \sqrt{-11b_2^2 + 36b_1|b_3|} \right). \tag{5.11}
$$

Note that since we are considering the nontrivial case  $|b_3| > b_2^2/(3b_1)$ , the expression in the square root of Eqs. [\(5.10\)](#page-6-2) and [\(5.11\)](#page-6-3) is positive and is greater than  $b_1$ , which also implies that the right-hand side of Eq.  $(5.11)$  is negative. In general, the inequality [\(5.9\)](#page-6-1) is a stronger condition than [\(5.6\)](#page-5-4)–[\(5.7\)](#page-5-3); for example, with  $b_3 < 0$  and  $|b_3| = b_2^2/b_1$ , it follows that  $(k_1^2)_{\text{min}} = 0$  in Eq. [\(5.7\),](#page-5-3) but [\(5.9\)](#page-6-1) yields the constraints that  $k_1 > |b_2|/b_1$  from [\(5.10\)](#page-6-2) or  $k_1 < -2|b_2|/(3b_1)$  from [\(5.11\).](#page-6-3)

Having shown that  $k_1$  can be chosen so that  $S_{R,2,k_1}$ satisfies conditions  $C_1$  and  $C_3$ , we next check conditions  $C_3$  and  $C_4$ . For this purpose, we need to analyze the inverse transformation, in which, for a given  $a$ , we calculate  $a'$  from the relation [\(2.6\)](#page-2-4). For  $S_{R,2,k_1}$ , Eq. [\(2.6\)](#page-2-4) is the cubic

$$
S_{R,2,k_1}: a = a' \left[ 1 + k_1 a' + \left( \frac{b_3}{b_1} + \frac{b_2}{b_1} k_1 + k_1^2 \right) (a')^2 \right].
$$
\n(5.12)

<span id="page-6-4"></span>As an illustrative case, we consider  $N_c = 3$  with  $N_f = 12$ , for which the two-loop beta function has a

(scheme-independent) zero at  $\alpha_{IR,2\ell} = \alpha'_{IR,2\ell} = 0.754$ , i.e.,  $a_{IR,2\ell} = a'_{IR,2\ell} = 0.060$ . We study the effect of carrying out the scheme transformation  $S_{R,2,k_1}$  on the beta function. From our general results above, we calculate  $|\bar{k}_1|_{\text{min}} = 0.692$  to satisfy  $f(a') > 0$  and  $\bar{k}_1 >$ 1.525 or  $\overline{k}_1 < -1.08$  to satisfy  $J > 0$ . We choose  $\bar{k}_1 = 1.751$ . Substituting this into Eq. [\(2.6\)](#page-2-4) together with  $a = 0.060$  and solving for  $a'$ , we obtain, for the relevant physical root,  $a' = 0.0399$ , i.e.,  $\alpha' = 0.502$  [\[26\].](#page-13-10) (The other two roots of the cubic equation are  $a' = -0.0575$ , which is unphysical, and  $a' = 0.1107$ , which lies farther away from the origin than  $a' = 0.0399$  and hence is not reached in the evolution of the theory from the UV to the IR.) This moderate shift downward in the value of the IR zero  $\alpha'$  obtained by the  $S_{R,2,k_1}$  transformation is similar to the value of the IR zero that one obtains by staying within the MS scheme and calculating to three-loop order, namely,  $\alpha_{IR,3\ell} = 0.435$ . We have found similar results for other values of  $N_c$  and  $N_f$ . Thus, condition  $C_2$ is satisfied, since the  $S_{R,2,k_1}$  transformation with this value of  $k_1$  maps a moderate value of a to a moderate (smaller) value of  $a'$ . Condition  $C_4$  is also obviously satisfied. Continuity of the scheme transformation implies that for values of  $k_1$  close to this value, the same qualitative and quantitative results hold.

## <span id="page-6-0"></span>VI. APPLICATION OF THE  $S_{R,3,K_1}$  SCHEME TRANSFORMATION

<span id="page-6-5"></span>Next, we study the  $S_{R,3,k_1}$  scheme transformation. The transformation function  $f(a')$  for  $S_{R,3,k_1}$  is

$$
S_{R,3,k_1}: f(a') = 1 + k_1 a' + k_2 (a')^2 + k_3 (a')^3, \quad (6.1)
$$

where  $k_2$  and  $k_3$  are given by Eqs. [\(3.5\)](#page-3-3) and [\(3.6\)](#page-3-4). From the  $m = 3$  special case of Eq. [\(3.3\),](#page-3-5) it follows that after the application of the  $S_{R,3}$  scheme transformation, in terms of the new variable  $\alpha'$ ,

$$
\alpha'_{\text{IR},4\ell} = \alpha'_{\text{IR},3\ell} = \alpha'_{\text{IR},2\ell} = \alpha_{\text{IR},2\ell}.\tag{6.2}
$$

We again assume that  $N_f \in I$ , so that the two-loop beta function has an IR zero. Evaluating  $f(a')$  at this (schemeindependent) two-loop zero,  $a'_{IR,2\ell} = a_{IR,2\ell} = -b_1/b_2$ , we have

$$
S_{R,3,k1}: f(a'_{IR,2\ell}) = 1 + \frac{b_1 b_3}{b_2^2} - \frac{b_1^2 b_4}{2b_2^3} - 3\frac{b_1^2 b_3}{b_2^3} k_1 - \frac{3b_1^2}{2b_2^2} k_1^2 - \frac{b_1^3}{b_2^3} k_1^3. \tag{6.3}
$$

An important property of Eq. [\(6.3\)](#page-6-4) is that the coefficient of the highest-degree term,  $k_1^3$ , is positive, namely,  $-(b_1/b_2)^3 = (b_1/|b_2|)^3$ . In [\[3\],](#page-12-2) it was shown that for  $S_{R,3} = S_{R,3,0}$ , i.e., if  $k_1 = 0$ ,  $f(a'_{\text{IR},2\ell})$  can be negative, violating condition  $C_1$ . In contrast, with nonzero  $k_1$ , because the coefficient of the highest power of  $k_1$  in [\(6.3\)](#page-6-4) is positive, we can always satisfy the inequality by using a sufficiently large value of  $k_1$ .

We next consider condition  $C_3$ , that  $J > 0$ . Evaluating J at  $a'_{IR,2l} = a_{IR,2l}$ , we find

$$
S_{R,3,k1}: J = 1 + \frac{3b_1b_3}{b_2^2} - \frac{2b_1^2b_4}{b_2^3} + \left(\frac{b_1}{b_2} - \frac{12b_1^2b_3}{b_2^3}\right)k_1 - \frac{7b_1^2}{b_2^2}k_1^2 - \frac{4b_1^3}{b_2^3}k_1^3. \tag{6.4}
$$

Again, the coefficient of the highest-degree (degree 3) term in  $k_1$  is positive, namely,  $-4(b_1/b_2)^3 = 4(b_1/|b_2|)^3$ . Hence, we can choose  $k_1$  so as to guarantee that  $J > 0$  for  $N_f \in I$ .

We generalize these results for  $S_{R,2,k_1}$  and  $S_{R,3,k_1}$  as follows. We find that for the  $S_{R,m,k_1}$  transformation, the respective highest-degree terms in the variable  $k_1$  in  $f(a')$ and *J* evaluated at  $a'_{\text{IR},2\ell}$  have degree *m* and have positive coefficients  $\alpha$   $(-1)^m (b_1/b_2)^m = (b_1/|b_2|)^m$ . Therefore, by choosing  $k_1$  appropriately, one can always render both  $f(a')$  and J evaluated at  $a'_{\text{IR},2\ell}$  positive. This contrasts with the simpler scheme transformations  $S_{R,m}$  =  $S_{R,m,0}$  which were analyzed in [\[2,3\]](#page-12-1) and were shown not to satisfy conditions  $C_1$  and  $C_3$ . For values of a that are such that we trust perturbation theory, the location of the IR zero in  $\beta_{n\ell}$  for  $n \geq 3$  should not differ very much from the value in  $\beta_{2\ell}$ , so by a continuity argument, it follows that it is possible to choose a  $k_1$  that again guarantees that  $f(a')$  and J are positive. In this range of values of a, all of the conditions  $C_1$  through  $C_4$  are satisfied.

As noted before, the maximum  $m$  for which we can explicitly analyze the application of the  $S_{R,m,k_1}$  scheme transformation in an asymptotically free theory is  $m = 3$ , because this requires knowledge of the  $b<sub>f</sub>$  for  $1 \leq \ell \leq m+1$ , and the  $b_{\ell}$  have only been computed up to  $m = 4$  loops. Nevertheless, it is of interest to calculate the coefficients  $b'_{\ell}$  resulting from the application of the  $S_{R,4,k_1}$  scheme transformation, and we have done this.

## <span id="page-7-0"></span>VII. SCHEME TRANSFORMATIONS IN THE LIMIT  $N_c \to \infty$ ,  $N_f \to \infty$  WITH  $N_f/N_c$  FIXED

#### A. General

One can get further insight into the application of the  $S_{R,2,k_1}$  and  $S_{R,3,k_1}$  scheme transformations at an IR zero of the beta function by considering an  $SU(N_c)$  gauge theory with  $N_f$  fermions in the fundamental representa-tion and taking the limit [\[28\]](#page-13-14)  $N_c \rightarrow \infty$  and  $N_f \rightarrow \infty$ with the ratio

$$
r \equiv \frac{N_f}{N_c},\tag{7.1}
$$

held fixed and finite. One also imposes the condition that the products

$$
x(\mu) \equiv N_c a(\mu), \qquad \xi(\mu) \equiv N_c a(\mu) = 4\pi x(\mu), \quad (7.2)
$$

should be fixed, finite functions of  $\mu$  in this limit. (As before, we will often suppress the argument  $\mu$  in the notation.) We call this the LNN (large  $N_c$  and  $N_f$ ) limit.

As in [\[20\]](#page-13-15), to have a beta function that has a finite, nontrivial LNN limit, we multiply both sides of Eq. [\(2.2\)](#page-1-1) by  $N_c$  and define

$$
\beta_{\xi} \equiv \frac{d\xi}{dt} = \lim_{\text{LNN}} \beta_a N_c. \tag{7.3}
$$

<span id="page-7-1"></span>This has the power series expansion

$$
\beta_{\xi} \equiv \frac{d\xi}{dt} = -8\pi x \sum_{\ell=1}^{\infty} \hat{b}_{\ell} x^{\ell} = -2\xi \sum_{\ell=1}^{\infty} \tilde{b}_{\ell} \xi^{\ell},\qquad(7.4)
$$

and

$$
\hat{b}_{\ell} = \lim_{\text{LNN}} \frac{b_{\ell}}{N_c^{\ell}}, \qquad \tilde{b}_{\ell} = \lim_{\text{LNN}} \frac{\bar{b}_{\ell}}{N_c^{\ell}}.
$$
\n(7.5)

We define the *n*-loop  $\beta_{\xi}$  function by Eq. [\(7.4\)](#page-7-1) 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

$$
\hat{b}_1 = \frac{11 - 2r}{3}, \qquad \hat{b}_2 = \frac{34 - 13r}{3}.
$$
\n(7.6)

To maintain asymptotic freedom, one restricts  $r < 11/2$ . We will focus on the interval  $r \in I_r$  where  $\beta_{\xi,2\ell}$  has an IR zero, namely,

$$
I_r: \frac{34}{13} < r < \frac{11}{2},\tag{7.7}
$$

i.e.,  $2.615 < r < 5.500$ . This zero occurs at

$$
x_{\text{IR},2\ell} = \frac{11 - 2r}{13r - 34}.
$$
 (7.8)

We have [\[20\]](#page-13-15)

$$
\hat{b}_3 = \frac{1}{54} (2857 - 1709r + 112r^2)
$$
  
= 52.9074 - 31.6481r + 2.07407r<sup>2</sup> (7.9)

and

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$$
\hat{b}_4 = \frac{150473}{486} - \left(\frac{485513}{1944}\right)r + \left(\frac{8654}{243}\right)r^2 + \left(\frac{130}{243}\right)r^3 + \frac{4}{9}\left(11 - 5r + 21r^2\right)\zeta(3)
$$
\n
$$
= 315.492 - 252.421r + 46.832r^2 + 0.534979r^3,\tag{7.10}
$$

to the indicated numerical floating-point accuracy, where  $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$  is the Riemann  $\zeta$  function, with  $\zeta(3) = 1.202057.$ 

A scheme transformation in this LNN limit has the form  $x = x'f(x')$ . We impose the condition that  $f(0) = 1$  to keep the properties of the theory the same as the coupling goes to zero. Using an  $f(x')$  that is analytic at  $x' = x = 0$ , we have the expansion

$$
f(x') = 1 + \sum_{s=1}^{s_{\text{max}}} \hat{k}_s(x')^s = 1 + \sum_{s=1}^{s_{\text{max}}} \hat{k}_s(\xi')^s, \qquad (7.11)
$$

where the  $\hat{k}_s$  and  $\hat{k}_s$  are given by the expressions for the  $k_s$ and  $\bar{k}_s$  with the various  $\bar{b}_n$  coefficients replaced by  $\hat{b}_n$ . The Jacobian is

$$
J = \frac{da}{da'} = \frac{dx}{dx'} = 1 + \sum_{s=1}^{s_{\text{max}}} (s+1)\hat{k}_s(x')^s
$$
  
=  $1 + \sum_{s=1}^{s_{\text{max}}} (s+1)\hat{k}_s(\xi')^s.$  (7.12)

We will denote the scheme transformation on  $x$  in the LNN limit that corresponds to  $S_{R,m,k_1}$  with the rescalings indicated above as  $S_{R,m,\hat{k}_1;LNN}$ . We construct the scheme transformation  $S_{R,m,\hat{k}_1;LNN}$  in the same way that we constructed  $S_{R,m,k_1}$ , by solving the equations for  $\tilde{b}_{\ell} = 0$  for  $3 \leq \ell \leq m + 1$ .

# B.  $S_{R,2,\hat{k}_1;LNN}$  scheme transformation

<span id="page-8-1"></span>For the  $S_{R,2,\hat{k}_1;LNN}$  scheme transformation, we calculate

$$
\hat{k}_2 = \frac{\hat{b}_3}{\hat{b}_1} + \frac{\hat{b}_2}{\hat{b}_1}\hat{k}_1 + \hat{k}_1^2
$$
  
= 
$$
\frac{2857 - 1709r + 112r^2}{18(11 - 2r)} - \left(\frac{13r - 34}{11 - 2r}\right)\hat{k}_1 + \hat{k}_1^2.
$$
  
(7.13)

<span id="page-8-0"></span>Evaluating the  $S_{R,2,\hat{k}_1;LNN}$  expression for  $f(x')$  at  $x = x_{IR,2\ell}$ , we calculate

$$
S_{R,2,\hat{k}_1;LNN}: f(x'_{IR,2\ell}) = 1 + \hat{k}_1 x'_{IR,2\ell} + \hat{k}_2 (x'_{IR,2\ell})^2
$$
  
=  $1 + \frac{\hat{b}_1 \hat{b}_3}{\hat{b}_2^2} + \frac{\hat{b}_1^2}{\hat{b}_2^2} k_1^2$   
=  $\frac{52235 - 40425r + 7692r^2 - 224r^3}{18(13r - 34)^2}$   
+  $\left(\frac{11 - 2r}{13r - 34}\right)^2 \hat{k}_1^2$ . (7.14)

In [\[3\]](#page-12-2) we showed that for the case  $k_1 = \hat{k}_1 = 0$ , i.e., the  $S_{R,2}$  scheme transformation, and  $r \in I_r$ ,  $f(x'_{IR,2\ell})$  is negative for  $34/13 < r < 4.07$  and positive for  $4.07 <$  $r < 11/2$  (to the indicated floating-point numerical accuracy). Here, by choosing nonzero  $\hat{k}_1$ , we can enlarge the range over which  $f(x'_{IR,2\ell}) > 0$ , satisfying condition  $C_1$ . The lower bound on  $\hat{k}_1^2$  such that this positivity holds is

$$
(\hat{k}_1^2)_{\min} = \frac{-52235 + 40425r - 7692r^2 + 224r^3}{18(11 - 2r)^2}.
$$
 (7.15)

For example, for a value roughly in the middle of the interval  $I_r$ , namely,  $r = 4$ , for which  $x_{IR,2\ell} = 1/6$ , this condition is that  $|\hat{k}_1| > 2.12$ .

The Jacobian for the  $S_{R,2,\hat{k}_1;LNN}$  scheme transformation, evaluated at  $x' = x'_{IR,2\ell} = -\hat{b}_1/\hat{b}_2$ , is

$$
S_{R,2,\hat{k}_1;LNN}: J = 1 + \frac{3\hat{b}_1\hat{b}_3}{\hat{b}_2^2} + \frac{\hat{b}_1}{\hat{b}_2}\hat{k}_1 + \frac{3\hat{b}_1^2}{\hat{b}_2^2}\hat{k}_1^2
$$
  
= 
$$
\frac{38363 - 29817r + 5664r^2 - 224r^3}{6(13r - 34)^2}
$$

$$
-\left(\frac{11 - 2r}{13r - 34}\right)\hat{k}_1 + 3\left(\frac{11 - 2r}{13r - 34}\right)^2\hat{k}_1^2.
$$
(7.16)

If  $\hat{k}_1 = 0$ , i.e., for the  $S_{R,2}$  scheme transformation, and with  $r \in I_r$ , this J is negative for  $34/13 < r < 4.69$  and positive for  $4.69 < r < 11/2$ . Here, with the  $S_{R,2,k_1}$  scheme transformation, we can choose  $\hat{k}_1$  to render J positive throughout all of the interval  $I_r$ , as required by condition  $C_3$ . We can do this because the coefficient of the term in J of highest degree in  $\hat{k}_1$  (namely, degree 2) is positive. We find that  $J > 0$  if

$$
\hat{k}_1 > \frac{13r - 34 + (-75570 + 58750r - 11159r^2 + 448r^3)^{1/2}}{6(11 - 2r)}
$$
\n(7.17)

or

$$
\hat{k}_1 < \frac{13r - 34 - (-75570 + 58750r - 11159r^2 + 448r^3)^{1/2}}{6(11 - 2r)}.
$$
\n(7.18)

For example, for a value roughly in the middle of the interval  $I_r$ ,  $r = 4$ , these inequalities are  $\hat{k}_1 > 6.43$  or  $\hat{k}_1 < -4.43$  (i.e.,  $\hat{k}_1 > 0.512$  or  $\hat{k}_1 < -0.353$ ). To check conditions  $C_2$  and  $C_4$ , we first pick  $\hat{k}_1 = 7$  (i.e.,  $\hat{k}_1 = 0.557$  and substitute this into the equation  $x =$  $x'f(x')$  for this  $S_{R,2,\hat{k}_1;LNN}$  transformation, which is a cubic equation for x'. Setting x equal to the value  $x_{\text{IR},2\ell} = 1/6$  for  $r = 4$ , and solving for x', we get, as the relevant physical root,  $x' = 0.123$ . This is similar to, and slightly smaller than,  $x = 1/6 = 0.167$ . (The other two roots of the cubic equation are  $x' = -0.163$ , which is unphysical, and  $x' = 0.2485$ , which is farther from the origin than  $x' = 0.123$  and hence is not reached in the evolution of the coupling from the UV to IR.) For comparison, we pick  $\hat{k}_1 - 6$  and follow the same procedure. This yields the relevant physical root  $x' = 0.179$ , slightly larger than 1/6. For both of these choices of  $\hat{k}_1$ , all of the acceptability conditions are satisfied.

# C.  $S_{R,3,\hat{k}_1;LNN}$  scheme transformation

The  $S_{R,3,\hat{k}_1;LNN}$  scheme transformation has the same  $\hat{k}_2$  as the  $S_{R,2,\hat{k}_1;LNN}$  transformation, given above in Eq. [\(7.13\)](#page-8-1). For  $\hat{k}_3$ , we calculate

$$
\hat{k}_3 = \frac{\hat{b}_4}{2\hat{b}_1} + \frac{3\hat{b}_3}{\hat{b}_1}\hat{k}_1 + \frac{5\hat{b}_2}{2\hat{b}_1}\hat{k}_1^2 + \hat{k}_1^3
$$
\n
$$
= \frac{1}{6^4(11 - 2r)}[601892 - 485513r + 69232r^2 + 1040r^3
$$
\n
$$
+ \zeta(3)(9504 - 4320r + 18144r^2)]
$$
\n
$$
+ \frac{(2857 - 1709r + 112r^2)\hat{k}_1}{6(11 - 2r)} - \frac{5(13r - 34)\hat{k}_1^2}{2(11 - 2r)} + \hat{k}_1^3.
$$
\n(7.19)

The  $S_{R,3,\hat{k}_1;LNN}$  expression for  $f(x')$  evaluated at  $x =$  $x_{IR,2\ell}$  is given by the right-hand side of Eq. [\(6.1\)](#page-6-5) with the  $b_{\ell}$ replaced by  $\hat{b}_{\ell}$  with  $1 \leq \ell \leq 4$ . Substituting the above expressions for these, we obtain

<span id="page-9-0"></span>
$$
S_{R,3,\hat{k}_1; \text{LNN}} \Rightarrow f(x'_{\text{IR},2\ell}) = \frac{1}{6^4 (13r - 34)^3} \left[ -55042348 + 62622039r - 24520604r^2 + 2885644r^3 + 21504r^4 + 4160r^5 + \zeta(3)(1149984 - 940896r + 2423520r^2 - 815616r^3 + 72576r^4) \right] + \frac{(11 - 2r)^2 (2857 - 1709r + 112r^2)\hat{k}_1}{6(13r - 34)^3} - \frac{3}{2} \left( \frac{11 - 2r}{13r - 34} \right)^2 \hat{k}_1^2 + \left( \frac{11 - 2r}{13r - 34} \right)^3 \hat{k}_1^3. \tag{7.20}
$$

<span id="page-9-1"></span>With the same substitution  $x' = x'_{IR,2\ell}$  in J, we get

$$
S_{R,3,\hat{k}_1; \text{LNN}} \Rightarrow J = 1 + \frac{(11 - 2r)(2857 - 1709r + 112r^2)}{6(13r - 34)^2} + \frac{(11 - 2r)^2}{324(13r - 34)^3} [601892 - 485513r + 69232r^2 + 1040r^3 + \zeta(3)(9504 - 4320r + 18144r^2)] + \frac{(11 - 2r)(59386 - 46374r + 8793r^2 - 448r^3)\hat{k}_1}{3(13r - 34)^3} - 7\left(\frac{11 - 2r}{13r - 34}\right)^2 \hat{k}_1^2 + 4\left(\frac{11 - 2r}{13r - 34}\right)^3 \hat{k}_1^3. \tag{7.21}
$$

If  $\hat{k}_1 = 0$ , then for  $r \in I_r$ ,  $f(x'_{IR,2\ell})$  is negative for  $34/13 < r < 3.95$  and positive for  $3.95 < r < 11/2$ , while J is negative for  $34/13 < r < 4.58$  and positive for  $4.58 < r < 11/2$ . Since the coefficients of the  $\hat{k}_1^3$  terms in Eqs. [\(7.20\)](#page-9-0) and [\(7.21\)](#page-9-1) are positive, we can choose  $\hat{k}_1$ appropriately to enlarge the region of  $r \in I_r$  for which  $f(x_{IR,2\ell})$  and J are positive, so that conditions  $C_1$  and  $C_3$ are satisfied. For example, for the value  $r = 4$ , roughly in the middle of the interval  $I_r$ ,  $f(x'_{IR,2\ell})$  in Eq. [\(7.20\)](#page-9-0) is positive for  $\hat{k}_1 > 1.30$  or  $-0.597 < \hat{k}_1 < 0.0115$ , while J in Eq. [\(7.21\)](#page-9-1) is positive for  $\hat{k}_1 > 1.43$  or  $-0.543 < \hat{k}_1 <$  $-0.0541$ . Recall that for  $r = 4$ ,  $x_{IR,2\ell} = 1/6$ . Setting  $\hat{k}_1 =$  $-0.199$  in  $f(x')$  for the  $S_{R,3,\hat{k}_1;LNN}$  scheme transformation

and solving the quartic equation  $x = x'f(x')$  for this  $S_{R,3,\hat{k}_1;LNN}$  transformation, we find  $x'=0.157$ , close to and slightly smaller than  $x_{IR,2\ell}$ . (The other three roots of the quartic equation are all unphysical, namely  $x' = -0.190$ and  $x' = 0.569 \pm 0.142i$ .) As is evident, conditions  $C_2$  and  $C_4$  are thus also satisfied. Again, one can use a continuity argument to infer that the same conclusion holds for neighboring values of r and  $\hat{k}_1$ . Thus, as we did for finite  $N_c$  and  $N_f \in I$ , here, in the LNN limit with  $r \in I_r$ , we have shown that, by the use of the parameter  $\hat{k}_1$  in the  $S_{R,2,\hat{k}_1;LNN}$ and  $S_{R,3,\hat{k}_1;LNN}$  scheme transformations, we can enlarge the region of applicability of these transformations as compared with the respective transformations with  $\hat{k}_1 = 0$ studied in [\[2,3\]](#page-12-1).

#### VIII. ON A MODIFIED  $S_1$  SCHEME TRANSFORMATION

<span id="page-10-0"></span>Here we present a modification of the scheme transition denoted  $S_1$  in [\[2\]](#page-12-1) which was designed to remove the threeloop term in the beta function. This scheme transformation has  $s_{\text{max}} = 1$  and thus has the form  $a = a'(1 + k_1 a')$ . Solving this quadratic equation for  $a'$  formally yields two solutions, but only one is physical, namely

$$
a' = \frac{1}{2k_1}(-1 + \sqrt{1 + 4k_1a}),\tag{8.1}
$$

since only this solution has the property that  $a \rightarrow a'$  as  $a \rightarrow 0$ . Since the purpose of this transformation is to render  $b'_3 = 0$ , this condition is used to determine  $k_1$ . The condition  $b'_3 = 0$  in this case is the equation  $b_3 + k_1b_2 +$  $k_1^2 b_1 = 0$ . In contrast to the  $S_{R,m,k_1}$  scheme transformation, for which all of the equations for the  $k<sub>s</sub>$  with  $s \ge 2$  are linear, this equation is quadratic and has the two formal solutions

<span id="page-10-3"></span>
$$
k_{1p}, k_{1m} = \frac{1}{2b_1} \left( -b_2 \pm \sqrt{b_2^2 - 4b_1b_3} \right), \tag{8.2}
$$

where the p, m subscripts refer to the  $\pm$  sign in Eq. [\(8.2\)](#page-10-3). If one requires that this scheme transformation must obey the conditions  $C_1$ - $C_4$  throughout all of the interval I, then the only acceptable choice is  $k_1 = k_{1p}$ , as was shown in [\[2\]](#page-12-1). The application of the  $S_1$  scheme transformation with this choice was analyzed in [\[2\].](#page-12-1) The regime of  $N_f$  values for which the  $S_1$  transformation with  $k = k_{1m}$  is unacceptable is toward the lower end of the interval I, where the value of the IR zero,  $a_{IR,2\ell} = -4\pi b_1/b_2 = 4\pi b_1/b_2$ , gets large. In view of this, one could alternatively choose not to try to apply the scheme transformation to the lower end of the interval I, since one could plausibly consider that the coupling is too large there for perturbative methods to be reliable. In this approach, one could study the application of the scheme transformation  $S_1$  with the choice  $k_1 = k_{1m}$ instead of  $k_1 = k_{1p}$ .

We explore this alternative approach here. With  $b_3 < 0$ , we reexpress  $k_{1m}$  in terms of positive quantities as

$$
k_{1m} = \frac{1}{2b_1} \left[ |b_2| - \sqrt{b_2^2 + 4b_1|b_3|} \right].
$$
 (8.3)

If we restrict the application of the  $S_1$  scheme transformation to the middle and upper parts of the interval *I*, then the choice  $k_1 = k_{1m}$  actually has an advantage as compared with the choice  $k_1 = k_{1p}$ . This can be shown as follows. We recall that as  $N_f$  approaches  $N_{f,b1z}$ ,  $b_1$  gets small and, consequently,  $k_{1p}$  can become somewhat large. This growth in  $k_{1p}$  is canceled in the  $S_1$  transformation, because  $k_{1p}$  multiplies a', and a and a' both approach zero in this limit. However, this does lead to some residual scheme dependence in the comparison between the fourloop IR zero in the MS scheme and the four-loop zero computed by applying this  $S_1$  scheme transformation to that scheme, as discussed in [\[2\].](#page-12-1) In contrast, with the sign choice  $k_1 = k_{1m}$ , as  $N_f$  increases toward  $N_{f,b1z}$ ,  $k_{1m}$ approaches  $-|b_3|/|b_2|$ , and hence its magnitude does not become large. Then, taking into account that  $a_{IR,2\ell}$ approaches zero in this limit, the inversion of the  $S_1$  scheme transformation with  $k_1 = k_{1m}$  yields values of a' that are closer to the corresponding values of  $a$  in this limit than was the case with the  $k_{1p}$  choice. Thus, the  $k_{1p}$  and  $k_{1m}$  choices have complementary advantages for the analysis of the IR zero with  $N_f \in I$  in these theories.

#### IX. CONCLUSIONS

<span id="page-10-1"></span>Because terms at loop order  $l \geq 3$  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 with sufficiently many fermions. In this paper, we have presented a generalized class of one-parameter scheme transformations, denoted  $S_{R,m,k_1}$  with  $m \geq 2$ , depending on a parameter  $k_1$ . A scheme transformation in this class eliminates the  $\ell$ -loop terms in the beta function from loop order  $l = 3$  to order  $l = m + 1$ , inclusive. We have analyzed the application of this class of scheme transformations to the infrared zero of the beta function of a non-Abelian  $SU(N_c)$  gauge theory with  $N_f$  fermions in the fundamental representation and have shown that an  $S_{R,m,k_1}$  scheme transformation in this class can satisfy the criteria to be physically acceptable over a larger range of  $N_f$  than the  $S_{R,m}$  transformation with  $k_1 = 0$ . As part of this, we have studied the properties of the corresponding scheme transformations in the limit  $N_c \rightarrow \infty$  and  $N_f \rightarrow \infty$  with  $N_f/N_c$  fixed and finite. We have also presented and discussed a modification of the  $S_1$ scheme transformation that removes the three-loop term in the beta of this theory. Our applications of the generalized scheme transformation provide a quantitative measure of the scheme dependence of the infrared fixed point of an asymptotically free non-Abelian gauge theory, adding to the results in [\[2,3\].](#page-12-1) These results are useful for the study of the UV to IR evolution of an asymptotically free gauge theory and, in particular, the investigation of the properties of a theory of this type with an infrared fixed point.

## ACKNOWLEDGMENTS

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#### <span id="page-10-2"></span>APPENDIX A: BETA FUNCTION COEFFICIENTS

For reference, we list the one-loop and two-loop coefficients  $[4-6]$  $[4-6]$  in the beta function  $(2.2)$  for a non-Abelian vectorial gauge theory with gauge group G and  $N_f$  Dirac fermions transforming according to the representation R:

$$
b_1 = \frac{1}{3} (11C_A - 4T_f N_f), \tag{A1}
$$

<span id="page-11-0"></span>
$$
b_2 = \frac{1}{3} [34C_A^2 - 4(5C_A + 3C_f)T_f N_f].
$$
 (A2)

(See Eq. (2.3) [\[29\].](#page-13-16)) Our calculations also make use of the three-loop and four-loop coefficients  $b_3$  and  $b_4$  calculated  $[9,10]$  in the  $\overline{\text{MS}}$  scheme.

## <span id="page-11-1"></span>APPENDIX B: EQUATIONS FOR THE  $b'_\ell$ RESULTING FROM A GENERAL SCHEME TRANSFORMATION

<span id="page-11-2"></span>The expressions for the  $b'_\ell$  in Eq. [\(2.10\)](#page-2-0) for  $3 \le \ell \le 6$ are [\[2\]](#page-12-1)

$$
b'_3 = b_3 + k_1 b_2 + (k_1^2 - k_2) b_1, \tag{B1}
$$

<span id="page-11-3"></span>
$$
b_4' = b_4 + 2k_1b_3 + k_1^2b_2 + (-2k_1^3 + 4k_1k_2 - 2k_3)b_1,
$$
\n(B2)

$$
b'_5 = b_5 + 3k_1b_4 + (2k_1^2 + k_2)b_3 + (-k_1^3 + 3k_1k_2 - k_3)b_2 + (4k_1^4 - 11k_1^2k_2 + 6k_1k_3 + 4k_2^2 - 3k_4)b_1,
$$
 (B3)

<span id="page-11-4"></span>and

$$
b'_6 = b_6 + 4k_1b_5 + (4k_1^2 + 2k_2)b_4 + 4k_1k_2b_3 + (2k_1^4 - 6k_1^2k_2 + 4k_1k_3 + 3k_2^2 - 2k_4)b_2
$$
  
+  $(-8k_1^5 + 28k_1^3k_2 - 16k_1^2k_3 - 20k_1k_2^2 + 8k_1k_4 + 12k_2k_3 - 4k_5)b_1.$  (B4)

The  $b'_\ell$  with  $\ell$  up to  $\ell = 8$  were given in [\[2\]](#page-12-1). As was noted in the text (with  $m + 1 = \ell$ ), a property that was used in our procedure for constructing the scheme transformation  $S_{R,m,k_1}$  is that in the expressions for  $b'_\ell$  with  $\ell \geq 3$ ,  $k_{\ell-1}$  occurs linearly, namely in the term  $-(\ell - 2)k_{\ell-1}b_1$ .

## APPENDIX C: HIGHER-ORDER COEFFICIENTS FOR  $S_{R,m,k_1}$

<span id="page-11-5"></span>In this appendix, we list expressions for some higher-order coefficients  $k_s$  in the  $S_{R,m,k_1}$  scheme transformation. We calculate that

$$
k_5 = \frac{b_6}{4b_1} - \frac{b_2b_5}{6b_1^2} + \frac{2b_3b_4}{b_1^2} + \frac{b_2^2b_4}{12b_1^3} - \frac{b_2b_3^2}{12b_1^3} + \left[\frac{5b_5}{3b_1} + \frac{7b_2b_4}{6b_1^2} + \frac{25b_3^2}{3b_1^2}\right]k_1 + \left[\frac{5b_4}{b_1} + \frac{27b_2b_3}{2b_1^2}\right]k_1^2 + \left[\frac{10b_3}{b_1} + \frac{35b_2^2}{6b_1^2}\right]k_1^3 + \left[\frac{77b_2}{12b_1}\right]k_1^4 + k_1^5 \quad \text{for } S_{R,m,k_1} \quad \text{with } \quad m \ge 5,
$$
\n
$$
(C1)
$$

and

$$
k_6 = \frac{b_7}{5b_1} - \frac{3b_2b_6}{20b_1^2} + \frac{8b_3b_5}{5b_1^2} + \frac{11b_4^2}{20b_1^2} - \frac{4b_2b_3b_4}{5b_1^3} + \frac{b_2^2b_5}{10b_1^3} + \frac{16b_3^3}{5b_1^3} + \frac{b_2^2b_3^2}{20b_1^4} - \frac{b_2^3b_4}{20b_1^4}
$$
  
+  $\left[\frac{3b_6}{2b_1} + \frac{2b_2b_5}{3b_1^2} + \frac{12b_3b_4}{b_1^2} + \frac{47b_2b_3^2}{6b_1^3} - \frac{b_2^2b_4}{3b_1^3}\right]k_1 + \left[\frac{5b_5}{b_1} + \frac{17b_2b_4}{2b_1^2} + \frac{25b_3^2}{b_1^2} + \frac{15b_2^2b_3}{2b_1^3}\right]k_1^2$   
+  $\left[\frac{10b_4}{b_1} + \frac{37b_2b_3}{b_1^2} + \frac{5b_3^3}{2b_1^3}\right]k_1^3 + \left[\frac{15b_3}{b_1} + \frac{85b_2^2}{6b_1^2}\right]k_1^4 + \left[\frac{87b_2}{10b_1}\right]k_1^5 + k_1^6 \text{ for } S_{R,m,k_1} \text{ with } m \ge 6. \quad (C2)$ 

# <span id="page-11-6"></span>APPENDIX D:  $b_\ell'$  COEFFICIENTS RESULTING FROM THE  $S_{R,2,k_1}$  SCHEME TRANSFORMATION

From the expressions for  $k_s$  in the  $S_{R,2,k_1}$  scheme transformation, we have calculated the resultant coefficients  $b'_\ell$  for  $\ell$  up to 8. We listed  $b'_e$  for  $e = 3,4, 5$  in Eqs. [\(4.1\)](#page-4-2)–[\(4.3\)](#page-4-1) in the text. Here we give the more lengthy expressions for the coefficients  $b'_{\ell}$  for  $\ell = 6, 7, 8$ . We have

$$
b'_6 = b_6 + \frac{2b_3b_4}{b_1} + \frac{3b_2b_3^2}{b_1^2} + \left[4b_5 + \frac{2b_2b_4}{b_1} - \frac{16b_3^2}{b_1} + \frac{6b_2^2b_3}{b_1^2}\right]k_1 + \left[6b_4 - \frac{36b_2b_3}{b_1} + \frac{3b_2^3}{b_1^2}\right]k_1^2 - \left[8b_3 + \frac{20b_2^2}{b_1}\right]k_1^3 - 13b_2k_1^4,
$$
\n(D1)

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$$
b'_{7} = b_{7} + \frac{3b_{3}b_{5}}{b_{1}} - \frac{9b_{3}^{3}}{b_{1}^{2}} + \left[5b_{6} + \frac{3b_{2}b_{5}}{b_{1}} + \frac{7b_{3}b_{4}}{b_{1}} - \frac{42b_{2}b_{3}^{2}}{b_{1}^{2}}\right]k_{1} + \left[10b_{5} + \frac{7b_{2}b_{4}}{b_{1}} + \frac{41b_{3}^{2}}{b_{1}} - \frac{57b_{2}^{2}b_{3}}{b_{1}^{2}}\right]k_{1}^{2} + \left[9b_{4} + \frac{69b_{2}b_{3}}{b_{1}} - \frac{24b_{2}^{3}}{b_{1}^{2}}\right]k_{1}^{3} + \left[44b_{3} + \frac{28b_{2}^{2}}{b_{1}}\right]k_{1}^{4} + 41b_{2}k_{1}^{5} + 9b_{1}k_{1}^{6},
$$
\n(D2)

and

$$
b'_{8} = b_{8} + \frac{4b_{3}b_{6}}{b_{1}} + \frac{4b_{3}^{2}b_{4}}{b_{1}^{2}} - \frac{8b_{2}b_{3}^{3}}{b_{1}^{3}} + \left[6b_{7} + \frac{4b_{2}b_{6}}{b_{1}} + \frac{12b_{3}b_{5}}{b_{1}} + \frac{8b_{2}b_{3}b_{4}}{b_{1}^{2}} + \frac{78b_{3}^{3}}{b_{1}^{2}} - \frac{24b_{2}^{2}b_{3}^{2}}{b_{1}^{3}}\right]k_{1} + \left[15b_{6} + \frac{12b_{2}b_{5}}{b_{1}} + \frac{12b_{3}b_{4}}{b_{1}} + \frac{4b_{2}^{2}b_{4}}{b_{1}^{2}} + \frac{258b_{2}b_{3}^{2}}{b_{1}^{2}} - \frac{24b_{2}^{3}b_{3}}{b_{1}^{3}}\right]k_{1}^{2} + \left[18b_{5} + \frac{18b_{3}^{2}}{b_{1}} + \frac{12b_{2}b_{4}}{b_{1}^{2}} + \frac{282b_{2}^{2}b_{3}}{b_{1}^{3}} - \frac{8b_{2}^{4}}{b_{1}^{3}}\right]k_{1}^{3} + \left[9b_{4} + \frac{64b_{2}b_{3}}{b_{1}} + \frac{102b_{2}^{3}}{b_{1}^{2}}\right]k_{1}^{4} + \left[-48b_{3} + \frac{46b_{2}^{2}}{b_{1}}\right]k_{1}^{5} - 42b_{2}k_{1}^{6} - 18b_{1}k_{1}^{7}.
$$
\n(D3)

# <span id="page-12-5"></span>APPENDIX E:  $b_\ell'$  COEFFICIENTS RESULTING FROM THE  $S_{R,3,k_1}$  SCHEME TRANSFORMATION

From the expressions for  $k_s$  in the  $S_{R,3,k_1}$  scheme transformation, we calculate the resultant  $b'_\ell$  coefficients. We obtain  $b'_3 = 0$ ,  $b'_4 = 0$ , and the result for  $b'_5$  given in Eq. [\(4.5\)](#page-4-3). For the  $b'_e$  with  $e'_6 = 6, 7, 8$ , we find

$$
b'_6 = b_6 + \frac{8b_3b_4}{b_1} + \frac{3b_2b_3^2}{b_1^2} + \left[4b_5 + \frac{10b_2b_4}{b_1} + \frac{20b_3^2}{b_1} + \frac{6b_2^2b_3}{b_1^2}\right]k_1 + \left[4b_4 + \frac{42b_2b_3}{b_1} + \frac{3b_2^3}{b_1^2}\right]k_1^2 + \left[-8b_3 + \frac{20b_2^2}{b_1}\right]k_1^3 - 7b_2k_1^4 - 4b_1k_1^5,
$$
\n(E1)

$$
b'_{7} = b_{7} + \frac{3b_{3}b_{5}}{b_{1}} + \frac{11b_{4}^{2}}{4b_{1}} - \frac{9b_{3}^{3}}{b_{1}^{2}} + \frac{9b_{2}b_{3}b_{4}}{2b_{1}^{2}} + \left[5b_{6} + \frac{3b_{2}b_{5}}{b_{1}} + \frac{10b_{3}b_{4}}{b_{1}} - \frac{15b_{2}b_{3}^{2}}{b_{1}^{2}} + \frac{9b_{2}^{2}b_{4}}{2b_{1}^{2}}\right]k_{1} + \left[10b_{5} + \frac{3b_{2}b_{4}}{b_{1}} - \frac{40b_{3}^{2}}{b_{1}} - \frac{15b_{2}^{2}b_{3}}{2b_{1}^{2}}\right]k_{1}^{2} + \left[10b_{4} - \frac{96b_{2}b_{3}}{b_{1}} - \frac{3b_{2}^{3}}{2b_{1}^{2}}\right]k_{1}^{3} - \left[10b_{3} + \frac{207b_{2}^{2}}{4b_{1}}\right]k_{1}^{4} - 17b_{2}k_{1}^{5}, \quad (E2)
$$

and

$$
b'_{8} = b_{8} + \frac{4b_{3}b_{6}}{b_{1}} + \frac{b_{4}b_{5}}{b_{1}} - \frac{18b_{3}^{2}b_{4}}{b_{1}^{2}} + \frac{7b_{2}b_{4}^{2}}{4b_{1}^{2}} - \frac{8b_{2}b_{3}^{3}}{b_{1}^{3}} + \left[6b_{7} + \frac{4b_{2}b_{6}}{b_{1}} + \frac{18b_{3}b_{5}}{b_{1}} - \frac{37b_{2}b_{3}b_{4}}{b_{1}^{2}} - \frac{54b_{3}^{3}}{b_{1}^{2}} - \frac{24b_{2}^{2}b_{3}^{2}}{b_{1}^{3}} - \frac{15b_{4}^{2}}{2b_{1}}\right]k_{1}
$$
  
+ 
$$
\left[15b_{6} + \frac{17b_{2}b_{5}}{b_{1}} - \frac{42b_{3}b_{4}}{b_{1}} - \frac{45b_{2}^{2}b_{4}}{2b_{1}^{2}} - \frac{185b_{2}b_{3}}{b_{1}^{2}} - \frac{24b_{2}^{3}b_{3}}{b_{1}^{3}}\right]k_{1}^{2} + \left[20b_{5} - \frac{26b_{2}b_{4}}{b_{1}} - \frac{80b_{3}^{2}}{b_{1}} - \frac{207b_{2}^{2}b_{3}}{b_{1}^{3}} - \frac{8b_{2}^{4}}{b_{1}^{3}}\right]k_{1}^{3}
$$
  
+ 
$$
\left[3b_{4} - \frac{116b_{2}b_{3}}{b_{1}} - \frac{297b_{3}^{3}}{4b_{1}^{2}}\right]k_{1}^{4} - \left[12b_{3} + \frac{89b_{2}^{2}}{2b_{1}}\right]k_{1}^{5} - 5b_{2}k_{1}^{6}.
$$
 (E3)

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