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<td>Lee, Weonjong.; Adams, David H.</td>
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Renormalization group evolution for the $\Delta S = 1$ effective Hamiltonian with $N_f = 2 + 1$

David H. Adams$^{1,\ast}$ and Weonjong Lee$^{2,\dagger}$

$^1$Department of Physics and Astronomy, Seoul National University, Seoul, 151-747, South Korea
$^2$Frontier Physics Research Division and Center for Theoretical Physics, Department of Physics and Astronomy, Seoul National University, Seoul, 151-747, South Korea

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We discuss the renormalization group (RG) evolution for the $\Delta S = 1$ operators in unquenched QCD with $N_f = 3$($m_u = m_d = m_s$) or, more generally, $N_f = 2 + 1$($m_u = m_d \neq m_s$) flavors. In particular, we focus on the specific problem of how to treat the singularities which show up only for $N_f = 3$ or $N_f = 2 + 1$ in the original solution of Buras et al. for the RG evolution matrix at next-to-leading order. On top of the original treatment of Buras et al., we use a new method of analytic continuation to obtain the correct solution in this case. It is free of singularities and can therefore be used in numerical analysis of data sets calculated in lattice QCD.

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I. INTRODUCTION

In the standard model, the direct CP violation parameter $\epsilon' / \epsilon$ and weak decays of hadrons are described by a low energy effective Hamiltonian which can be obtained by decoupling the heavy quarks and gauge bosons. In this paper, we consider the $\Delta S = 1$ effective Hamiltonian [1–5] which governs $\epsilon' / \epsilon$ and the $\Delta I = 1/2$ rule. The Hamiltonian is composed of hadronic matrix elements of four fermion operators with Wilson coefficients which are known up to next-to-leading order (NLO) in perturbation theory [2,6]. Since the energy scale in kaon decays is about 500 MeV, the hadronic matrix elements are dominated by the strong interaction, QCD. Hence, we must introduce a nonperturbative tool such as lattice gauge theory in order to calculate them [7–10].

Once we calculate the hadronic matrix elements on the lattice, we need to convert them into the corresponding quantities defined in a continuum renormalization scheme such as naive dimensional regularization (NDR); this is often called “matching.” When we match the lattice results to the continuum, we must introduce a matching scale $q^*$ [11]. A typical choice of $q^*$ lies in the range from $1/\alpha$ to $\pi/\alpha$ [12]. Once we match the lattice results to those in the continuum NDR scheme at the $q^*$ scale, we have two options to combine the Wilson coefficients with the continuum results. One is to run the hadronic matrix elements from $q^*$ down to $m$ ($N_f = 3$) and the other is to run the Wilson coefficients from $m$ up to $q^*$. To do this we use the renormalization group (RG) evolution equation at NLO, which is explained in great detail in [1–3]. In this paper we focus on the RG evolution equation and its solution at NLO.

For three sea quark flavors ($N_f = 3$ or $N_f = 2 + 1$), singularities arise in the NLO solution given in [1], even though the full RG evolution matrix is finite. This makes it impossible to calculate the RG evolution matrix numerically in this case, which is an essential step for the lattice evaluation of $\epsilon' / \epsilon$ and kaon decay amplitudes. Two unsatisfactory approaches to dealing with this problem have been attempted previously in the literature. In Refs. [7,13], the Wilson coefficients for $N_f = 3$ were combined with the hadronic matrix elements calculated using the RG evolution matrix with $N_f = 0$ (quenched QCD). In Refs. [8,14], the singularities were removed artificially by putting in an arbitrary cutoff of $\approx 1000$ by hand in the calculation of the $N_f = 3$ RG evolution matrix (i.e., singular matrix elements were replaced by finite ones with this value).

In this paper we provide the correct solution for this problem. Singularities do not arise, and it can therefore be used for numerical calculations. The applicability of our result is broad enough that any lattice calculation regardless of fermion discretization can take advantage of it. In fact, the results of this paper are already being used for the ongoing data analysis of the staggered $\epsilon' / \epsilon$ project [9,10].

Unquenched lattice simulations with $N_f = 2 + 1$ sea quark flavors are currently underway with a variety of fermion discretizations: AsqTad staggered fermions, HYP staggered fermions, Wilson clover fermions, twisted mass Wilson fermions, domain wall fermions, and overlap fermions (see, e.g., [15] and references therein). These simulations are currently focusing on decay constants ($f_\pi$ and $f_K$), hadron spectrum, the indirect CP violation parameter $B_K$, kaon semileptonic form factors, and kaon distribution amplitudes [15]. In the coming future, the simulations will be extended to address kaon physics such as $\epsilon' / \epsilon$ and the $\Delta I = 1/2$ rule. The results of this paper will be needed in connection with this.

This paper is organized as follows. In Sec. II, we review the RG evolution results originally presented in [1] and raise the serious problems for $N_f = 3$. In Sec. III, we provide the correct solution to the QCD part of the RG evolution equation, in which singularities do not arise. In
Sec. IV, we go on to present the correct solution to the QED part of the RG evolution equation, in which there are also no singularities. We close with some conclusions.

II. REVIEW OF RG EVOLUTION

The $\Delta S = 1$ effective Hamiltonian for nonleptonic decays may be written in general as

$$\mathcal{H}_{\text{eff}} = \frac{G_F}{\sqrt{2}} \sum_i C_i(\mu) \bar{q}(\mu) \frac{g}{\sqrt{2}} \mathcal{Q}_i(\mu) \cdot \mathcal{C}(\mu),$$

(1)

where the index $i$ runs over a basis for the contributing operators; in our example this is the basis $Q_1, Q_2, \ldots, Q_{10}$ of Buras et al. defined in Sec. 2 of Ref. [1]. The renormalization group equation for $\tilde{C}(\mu)$ is

$$\left[ \frac{\partial}{\partial \mu} + \beta(g) \frac{\partial}{\partial g} \right] \tilde{C} = \gamma^T(g, \alpha) \tilde{C},$$

(2)

where $\beta(g)$ is the QCD beta function:

$$\beta(g) = -\beta_0 \frac{g^3}{16\pi} - \beta_1 \frac{g^5}{(16\pi^2)^2} - \beta_{1c} \frac{e^2 g^3}{(16\pi)^2}$$

(3)

with

$$\beta_0 = 11 - \frac{2}{3} f \quad \beta_1 = 102 - \frac{38}{3} f \quad \beta_{1c} = -\frac{8}{9} \left( u + \frac{d}{4} \right)$$

(4)

and $f = u + d$ denoting the number of active flavors, and $u$ and $d$ being the number of $u$-type and $d$-type flavors, respectively. According to Buras et al., the contribution from the $\beta_{1c}$ term is negligible and they dropped it in Refs. [1,3]. We will include it here for the sake of completeness. The $\gamma(g, \alpha)$ matrix is the full $10 \times 10$ anomalous dimension matrix, which is given in [1].

The solution of the RG equation in Eq. (2) for the Wilson coefficient functions is given by

$$\tilde{C}(\mu) = U(\mu, \mu_w, \alpha) \tilde{C}(\mu_w).$$

(5)

The coefficients at the scale $\mu_w = \mathcal{O}(M_w)$ can be evaluated in perturbation theory. The evolution matrix $U$ then includes the renormalization group improved perturbative contributions from the scale $\mu_w$ down to $\mu$. For $m_1 < m_2$,

$$U(m_1, m_2, \alpha) = T_g \exp \left( \int_{g(m_2)}^{g(m_1)} dg' \frac{\gamma_T(g', \alpha)}{\beta(g')} \right).$$

(6)

where $g$ is the QCD coupling. Here, $T_g$ denotes ordering in the coupling constant such that the couplings increase from right to left. Note that for $g_1 \neq g_2$,

$$[\gamma(g_1), \gamma(g_2)] \neq 0.$$  

(7)

The evaluation of the amputated Green functions with insertion of the operators $\tilde{Q}$ gives the following relation:

$$\left\langle \tilde{Q} \right\rangle^{(0)} = Z_q \tilde{Z} \left\langle \tilde{Q} \right\rangle,$$

(8)

where $\left\langle \tilde{Q} \right\rangle^{(0)}$ and $\left\langle \tilde{Q} \right\rangle$ denote the unrenormalized and renormalized Green functions, respectively. $Z_q$ is the quark field renormalization constant and $\tilde{Z}$ is the renormalization constant matrix of the operators $\tilde{Q}$. The anomalous dimension matrices are defined by

$$\gamma(g, \alpha) = Z^{-1} \frac{d}{d \ln \mu} Z$$

(9)

which includes QCD and QED contributions. For the case at hand, $\gamma(g, \alpha)$ can be expanded in the following way (with $\alpha = \frac{e}{4\pi}$):

$$\gamma(g, \alpha) = \gamma_s(g^2) + \frac{\alpha_s}{4\pi} \gamma_s^0 + \frac{\alpha_s^2}{4\pi^2} \gamma_s^0 + \cdots.$$

(10)

The QCD part of the anomalous dimension, $\gamma_s$, can be expanded as (with $\alpha_s = \frac{e}{4\pi}$)

$$\gamma_s(g^2) = \frac{\alpha_s}{4\pi} \gamma_s^0 + \frac{\alpha_s^2}{4\pi^2} \gamma_s^0 + \cdots.$$  

(11)

The QED part of the anomalous dimension, $\Gamma$, can be expanded as

$$\Gamma(g^2) = \gamma_e^0 + \frac{\alpha_e}{4\pi} \gamma_e^0 + \cdots.$$  

(12)

The general RG evolution matrix $U(m_1, m_2, \alpha)$ of Eq. (6) may then be decomposed as follows:

$$U(m_1, m_2, \alpha) = U(m_1, m_2) + \frac{\alpha}{4\pi} R(m_1, m_2)$$

(13)

$$U(m_1, m_2) = T_g \exp \left( \int_{g(m_2)}^{g(m_1)} dg' \frac{\gamma_T(g', \alpha)}{\beta(g')} \right).$$

(14)

$$R(m_1, m_2) = \int_{g(m_2)}^{g(m_1)} dg' \frac{U(m_1, m') \Gamma(g') U(m', m_2)}{\beta(g')}.$$  

(15)

Here, $U(m_1, m_2)$ represents the pure QCD evolution and $R(m_1, m_2)$ describes the additional evolution in the presence of the electromagnetic interaction. The leading order RG equation describing the QED evolution was first discussed in [16].

The QCD evolution matrix which Buras et al. provided originally can be expressed up to NLO as

$$U(m_1, m_2) = \left( 1 + \frac{\alpha_s(m_1)}{4\pi} J \right) U^{(0)}(m_1, m_2) \left( 1 - \frac{\alpha_s(m_2)}{4\pi} J \right).$$

(16)

where $U^{(0)}(m_1, m_2)$ denotes the evolution matrix in the leading logarithmic approximation and $J$ summarizes the next-to-leading correction to this evolution. Additional terms proportional to $\alpha_s^2$ in $U(m_1, m_2)$ which do not come from $U^{(0)}(m_1, m_2)$ should be consistently dropped.
RENORMALIZATION GROUP EVOLUTION FOR THE ...

at NLO. Taking $V$ to be a matrix which diagonalizes $\gamma_s^{(0)T}$, we define the following:

$$\gamma_D^{(0)} = V^{-1} \gamma_s^{(0)T} V$$

(17)

$$G = V^{-1} \gamma_s^{(1)T} V,$$

(18)

where $\gamma_D^{(0)}$ denotes a diagonal matrix whose diagonal elements are the components of the vector $\tilde{\gamma}^{(0)}$. Then,

$$U^{(0)}(m_1, m_2) = V \left[ \begin{array}{c} \alpha_s(m_2) \\ \alpha_s(m_1) \end{array} \right] \gamma_D^{(0)} V^{-1}$$

(19)

with

$$\tilde{a} = \frac{\tilde{\gamma}^{(0)}}{2\beta_0}.$$  

(20)

For the matrix $J$, we find

$$J = VSV^{-1},$$

(21)

where the elements of $S$ are given by

$$S_{ij} = \delta_{ij} \gamma_i^{(0)} \frac{\beta_1}{2\beta_0} - \frac{G_{ij}}{2\beta_0 + \gamma_i^{(0)} - \gamma_j^{(0)}},$$

(22)

where $\gamma_i^{(0)}$ is a component of $\tilde{\gamma}^{(0)}$ and $G_{ij}$ denotes the elements of $G$ in Eq. (18). This is the result obtained by Buras et al. [1,3]. However, when $f = 3$ ($= N_f$), $i = 8$, and $j = 7$, the denominator of Eq. (22) vanishes: $2\beta_0 + \gamma_i^{(0)} - \gamma_j^{(0)} = 0$. Hence, the solution for the RG evolution matrix at NLO has singularities in this case, despite the fact that the full RG evolution matrix must be finite. This is one of the main issues we will address in this paper. This problem is briefly mentioned in [1,5] without any solution given. The correct treatment for this case, which is given in the next section, eradicates the singularities in Eqs. (16) and (22), and leads to a finite expression for the RG evolution matrix at NLO.

Next, we turn to the QED part of the evolution matrix $R(m_1, m_2)$ given in Eq. (15). We can expand $R(m_1, m_2)$ in powers of $g^2$ as follows:

$$R(m_1, m_2) = R^{(0)}(m_1, m_2) + R^{(1)}(m_1, m_2) + \cdots,$$

(23)

where $R^{(i)}$ is of the order of $g^{2i}$. It turns out to be convenient to introduce the matrix $K(m_1, m_2)$ to represent $R(m_1, m_2)$ as follows:

$$R(m_1, m_2) = -\frac{2\pi}{\beta_0} V K(m_1, m_2) V^{-1}$$

(24)

$$K(m_1, m_2) = K^{(0)}(m_1, m_2) + \frac{1}{4\pi} \sum_{i=1}^{3} K_i^{(1)}(m_1, m_2)$$

(25)

$$R^{(0)}(m_1, m_2) = -\frac{2\pi}{\beta_0} V K^{(0)}(m_1, m_2) V^{-1}$$

(26)

The leading order term can be obtained by straightforward integration

$$M^{(0)}(m_1, m_2) = \frac{M_{ij}^{(0)}}{\alpha_j - \alpha_i} \left[ \frac{\alpha_s(m_2)}{\alpha_s(m_1)} \right]^{a_i} \ln \left( \frac{\alpha_s(m_1)}{\alpha_s(m_2)} \right)$$

(28)

where the $a_i$’s are the components of $\tilde{a}$ in Eq. (20), and the $M^{(0)}$ matrix is given by

$$M^{(0)} = V^{-1} \gamma^{(0)T} V.$$  

(29)

Similar to the case of $S_{ij}$ in Eq. (22), there is a singularity in Eq. (28) for the element $(7, 8)$ of $(K^{(0)}(m_1, m_2))$ since $a_7 = a_8 + 1$ when $f = 3$ ($= N_f$). However, the expression in the numerator also vanishes in this case and so the singularity is removable. In this case of $a_i = a_j + 1$, direct integration leads to the following formula [1]:

$$K^{(0)}(m_1, m_2) = \frac{M^{(0)}}{\alpha_i(m_1)} \left[ \frac{\alpha_s(m_2)}{\alpha_s(m_1)} \right]^{a_j} \ln \left( \frac{\alpha_s(m_1)}{\alpha_s(m_2)} \right).$$

(30)

The next leading corrections to the QED part of the evolution matrix are represented by $K_i^{(1)}(m_1, m_2)$. We introduce

$$\Gamma^{(1)} = \gamma^{(0)T} - \frac{\beta_1}{\beta_0} \gamma^{(0)T} - \frac{\beta_{1e}}{\beta_0} \gamma^{(0)T}$$

(31)

and

$$M^{(1)}(m_1, m_2) = V^{-1} [\Gamma^{(1)} + [\gamma^{(0)T}, J] V].$$

(32)

The matrices $K_i^{(1)}(m_1, m_2)$ are then given as follows:

$$K_i^{(1)}(m_1, m_2) = M_i^{(1)} Q_{ij}$$

(33)

$$Q_{ij} = \begin{cases} 
\frac{1}{\alpha_1 - \alpha_i} \left[ \frac{(\alpha_s(m_2))^{a_j}}{(\alpha_s(m_1))^{a_j}} - \frac{(\alpha_s(m_2))^{a_i}}{(\alpha_s(m_1))^{a_i}} \right] & \text{if } i \neq j \\
\frac{(\alpha_s(m_2))^{a_i}}{(\alpha_s(m_1))^{a_i}} \ln \left( \frac{\alpha_s(m_1)}{\alpha_s(m_2)} \right) & \text{if } i = j 
\end{cases}$$

(34)

$$K_2^{(1)}(m_1, m_2) = -\alpha_s(m_2) K^{(0)}(m_1, m_2) S$$

(35)

$$K_3^{(1)}(m_1, m_2) = \alpha_s(m_1) S K^{(0)}(m_1, m_2).$$

(36)

As one can see in the above equations, all of the $K_i^{(1)}(m_1, m_2)$ matrices include $S$ or $J$. Since $S$ or $J$ is singular for $f = 3$ ($= N_f$), all the $K_i^{(1)}$ matrices are also singular. However, the full RG evolution matrix $R(m_1, m_2)$ must always be finite. The correct treatment of $R(m_1, m_2)$ at NLO in this case, given in Sec. IV, modifies the formulas
III. HOW TO HANDLE REMOVABLE SINGULARITIES FOR $N_f = 3$ (QCD PART)

For $f = 3$ (three dynamical flavors), when $i = 8$ and $j = 7$, $\beta_0 = 9$, $\gamma_i^{(0)} = -16$ and $\gamma_j^{(0)} = 2$. Hence, $2\beta_0 + \gamma_i^{(0)} - \gamma_j^{(0)} = 0$ corresponds to a pole in $S_{ij}$ of Eq. (22), which does not exist in the full evolution matrix and so should not appear in the correct solution at NLO. To find the latter, we start by rearranging the NLO expression for the QCD RG evolution matrix given in Eq. (16) as follows

$$U(m_1, m_2) = U_0(m_1, m_2) + \frac{1}{4\pi} VA(m_1, m_2)V^{-1},$$

where

$$VA(m_1, m_2)V^{-1} = \alpha_s(m_1)JU_0(m_1, m_2)$$

$$- \alpha_s(m_2)U_0(m_1, m_2)J.$$  

When $S$ and $J$ matrices are nonsingular, the $A$ matrix is readily found from Eqs. (19)–(22) and (38) to be given by

$$A_{ij} = S_{ij} \left[ \alpha_s(m_1) \left( \frac{\alpha_s(m_2)}{\alpha_s(m_1)} \right)^{a_i} - \alpha_s(m_2) \left( \frac{\alpha_s(m_2)}{\alpha_s(m_1)} \right)^{a_i} \right].$$

When $S_{ij}$ is singular (i.e. $i = 8$ and $j = 7$), this expression diverges and therefore cannot be used in numerical calculations. In this case, the correct finite expression for the $A$ matrix is

$$A_{ij} = \frac{G_{ij}}{2\beta_0} \alpha_s(m_2) \left( \frac{\alpha_s(m_2)}{\alpha_s(m_1)} \right)^{a_i} \ln \left( \frac{\alpha_s(m_2)}{\alpha_s(m_1)} \right).$$

The derivation is as follows. For $i \neq j$,

$$S_{ij} = \frac{G_{ij}}{2\beta_0(1 + a_i - a_j)}.$$  

We regularize the singularity that occurs when $a_j = a_i + 1$ ($i = 8$ and $j = 7$) by introducing an $\epsilon$ shift of $a_j$ so that $a_j = a_i + 1 + \epsilon$. Then

$$S_{ij} = \frac{G_{ij}}{2\beta_0} \frac{1}{\epsilon}$$

and $A_{ij}$ is given by

$$A_{ij} = \left( \frac{G_{ij}}{2\beta_0} \right) \epsilon \alpha_s(m_2) \left( \frac{\alpha_s(m_2)}{\alpha_s(m_1)} \right)^{a_i} \left[ \epsilon \ln \left( \frac{\alpha_s(m_2)}{\alpha_s(m_1)} \right) + O(\epsilon^2) \right].$$

In the limit of $\epsilon = 0$, we get the claimed result of Eq. (40).

The expression Eq. (40) is finite and can therefore be used for numerical calculations. In the Appendix we give an alternative derivation of this result, similar to the previous approach of Buras et al. in the nonsingular case [1,3,17].

IV. HOW TO HANDLE REMOVABLE SINGULARITIES FOR $N_f = 3$ (QED PART)

Now let us turn to the QED part of the evolution matrix for $f = 3$ ($= N_f$). Basically, we want to perform the integration on the right-hand side of Eq. (15). Equation (15) contains the QCD evolution matrix $U$. Since the $U$ matrix is modified due to the removable singularity for $f = 3$ as given in Eqs. (37)–(40), the QED part, the $R$ matrix, will also change correspondingly. In the following we provide this modified version of the $R$ matrix. As we mentioned in the previous section, we cannot use the $S$ and $J$ matrices because they are singular. Instead, we need to define a new matrix which is finite:

$$H_{ij} = S_{ij} \left( 1 - \delta_{i,8} \delta_{j,7} \right).$$

Note that the singular part is subtracted away so that the $H$ matrix is finite.

We now express the $R$ matrix as follows:

$$R(m_1, m_2) = -\frac{2\pi}{\beta_0} V \tilde{K}(m_1, m_2)V^{-1}$$

$$\tilde{K}(m_1, m_2) = K^{(0)}(m_1, m_2) + \frac{1}{4\pi} \sum_{i=1}^{4} \tilde{K}_{i}^{(1)}(m_1, m_2).$$

where the leading term $K^{(0)}$ is given in Eqs. (28)–(30). The $\tilde{K}_{i}^{(1)}$ matrices are given as

$$[\tilde{K}_{1}^{(1)}]_{ij} = [M^{(2)} + [M^{(0)}, H]]_{ij} Q_{ij}$$

$$[\tilde{K}_{2}^{(1)}]_{ij} = \alpha_s(m_1)[HK^{(0)}]_{ij}$$

$$[\tilde{K}_{3}^{(1)}]_{ij} = -\alpha_s(m_2)[K^{(0)}H]_{ij}$$

$$[\tilde{K}_{4}^{(1)}]_{ij} = \delta_{i8} \left( \frac{G_{87}M_{7j}^{(0)}}{2\beta_0} \right) [I_{1}]_{ij} + \delta_{j7} \left( \frac{M_{8i}^{(0)}G_{87}}{2\beta_0} \right) [I_{2}]_{ij},$$

where $M^{(2)}$ is

$$M^{(2)} = V^{-1} \Gamma^{(1)} V.$$
Note that the leading order contribution $K^{(0)}$ is the same as before. The only change is localized in the $K^{(1)}_i$ matrices. In particular, the $K^{(1)}_i$ matrices for $i = 1, 2, 3$ correspond to the $K^{(1)}$ matrices once we substitute the $S$ matrix by the $H$ matrix. The $K^{(1)}_4$ matrix represents the contribution from the removable singularity of the $S$ matrix. The key point is that the $K^{(1)}_i$ matrices are finite and can be used numerically, whereas the $K^{(1)}$ are divergent.

V. CONCLUSION

The original solution of Buras et al. for the RG evolution matrix at NLO contains removable singularities for $N_f = 3$, which cancel out in the proper combination. However, since the individual terms are singular, it is not possible to use it in the numerical calculation. In this paper, we provide the correct solution in which there are no singularities. Our results for both the QCD part and QED part of the RG evolution matrix are finite and can be used for numerical studies with $N_f = 2 + 1$. These results are currently being used to analyze the data sets of the staggered $\epsilon'/\epsilon$ project [18]. In fact, this work is a part of that project.

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APPENDIX: ALTERNATIVE DERIVATION OF THE PURE QCD EVOLUTION MATRIX AT NLO

In this Appendix we give an alternative derivation of the result for the pure QCD evolution matrix $U(m_1, m_2)$ at NLO in the singular case [Eqs. (37) and (40)]. Since the dependence of $U(m_1, m_2)$ on $m_i$ enters through $\alpha_i(m_i) = (g(m_i)/4\pi$, we will sometimes denote the evolution matrix by $U(g_1, g_2)$ when it is convenient. Following the earlier approach of Buras et al. [3,17], we express the evolution matrix as

$$U(g, g_0) = \left(1 + \frac{g^2}{16\pi^2} J(g)\right) U^{(0)}(g, g_0) \left(1 + \frac{g_0^2}{16\pi^2} J(g_0)\right)^{-1}$$

(A1)

and seek to determine $J(g)$ from the differential equation which characterizes $U(g, g_0)$:

$$\frac{d}{dg} U(g, g_0) = \frac{\gamma_f^2 (g^2)}{\beta(g)} U(g, g_0).$$

(A2)

Substituting (A1) into (A2), and introducing $S(g)$ via $J(g) = VS(g)V^{-1}$ as in Eq. (21), we find the following differential equation for the matrix elements of $S(g)$:

$$(2\beta_0 + \gamma_i^{(0)} - \gamma_j^{(0)}) S_{ij}(g) - \frac{g^2}{16\pi^2} \left(\frac{\beta_1}{\beta_0} \gamma_D^{(0)} G + O(g^2)\right) S_{ij} = \frac{\beta_1}{\beta_0} \gamma_i^{(0)} \delta_{ij} - G_{ij} + O(g^2).$$

(A3)

To solve this equation at leading order in $g$, it is necessary to consider separately the cases where $2\beta_0 + \gamma_i^{(0)} - \gamma_j^{(0)}$ is nonvanishing and vanishing. In the former case, a consistent solution is obtained at lowest order by taking $J(g) = J + O(g)$, where $J$ is a constant matrix. Then $S(g) = S + O(g)$, and the lowest order part of (A3) becomes

$$(2\beta_0 + \gamma_i^{(0)} - \gamma_j^{(0)}) S_{ij} = \frac{\beta_1}{\beta_0} \gamma_i^{(0)} \delta_{ij} - G_{ij}.$$  

(A4)

Dividing by $2\beta_0 + \gamma_i^{(0)} - \gamma_j^{(0)}$ gives the expression for $S_{ij}$ stated in Eq. (22), which was the one obtained previously by Buras et al. [3,17].
$\beta_0 g S_{ij}(g) = -G_{ij}$  \hspace{1cm} (A5)

which has the solution

$$S_{ij}(g) = -\frac{G_{ij}}{\beta_0} \log(g) + c_{ij}, \hspace{1cm} (A6)$$

where $c_{ij}$ is an undetermined integration constant. In fact, we do not need to determine $c_{ij}$ since it turns out not to contribute to the evolution matrix at NLO. To see this, recall that the evolution matrix is determined at NLO by $A(m_1, m_2)$ as in Eq. (37), where now

$$A(m_1, m_2) = \alpha_s(m_1) S(m_1) V^{-1} U^{(0)}(m_1, m_2) V - \alpha_s(m_2) V^{-1} U^{(0)}(m_1, m_2) VS(m_2). \hspace{1cm} (A7)$$

Reexpressing (A6) as

$$S_{ij}(m) = -\frac{G_{ij}}{2\beta_0} \log(\alpha_s(m)) + c'_{ij} \hspace{1cm} (A8)$$

[where $c'_{ij} = c_{ij} - \frac{G_{ij}}{2\beta_0} \log(4\pi)$] and substituting this into the expression for $A(m_1, m_2)_{ij}$ obtained from (A7) [recalling from Eqs. (19) and (20) that $V^{-1} U^{(0)}(m_1, m_2) V$ is diagonal], we easily find that the constant $c'_{ij}$ drops out and our previous expression [Eq. (40)] is reproduced. This completes the alternative derivation of the NLO expression for $U(m_1, m_2)$. The argument also shows that for calculations involving $U(m_1, m_2)$ at NLO we may take $S_{ij}$ in the singular case to be given by (A8) with $c'_{ij} \equiv 0$. This is useful for deriving the expressions [Eqs. (50)–(53)] for the QED part of the evolution matrix at NLO.