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Eradication of singularities in the next-to-leading order RG evolution for the $\Delta S = 1$ effective Hamiltonian with 3 quark flavours

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We consider the renormalization group (RG) evolution for the operators in the $\Delta S = 1$ effective Hamiltonian with 3 active quark flavors, which is needed in the numerical analysis of data sets for ε'/ε calculated in lattice QCD. Singularities are present in the original solution of Buras *et al.* at next-to-leading order (NLO). We show how these can be eradicated through a method of analytic continuation to obtain the correct finite solution in this case. Furthermore, we trace the origin of the singularities to a breakdown of the approach of Buras *et al.* in the 3 flavour case, and show how it can be rectified so that singularitites are absent from the beginning.

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1. Introduction

Weak $\Delta S = 1$ decays of hadrons can be described in the framework of the Standard Model by an effective Hamiltonian $\mathscr{H}_{eff}$ obtained by integrating out the degrees of freedom associated with heavy quarks and gauge bosons [1, 2, 3, 4, 5]. It governs interesting aspects of kaon physics; in particular the direct CP violation parameter ε'/ε and the $\Delta I = 1/2$ rule. The effective Hamiltonian has the form

$$\mathscr{H}_{eff} = \frac{G_F}{\sqrt{2}} \sum_i C_i(\mu, g, e) Q_i(\mu, g, e) \tag{1.1}$$

where $C_i(\mu, g, e)$ denotes the Wilson coefficients, the $Q(\mu, g, e)$'s are a basis of renormalized 4-fermion operators contributing to the effective Hamiltonian, μ is the scale, g the strong coupling and e the EM coupling. We take the basis operators Q_i to be the ones specified by Buras *et al.* in Section 2 of Ref.[1]. There are 10 of these and their origins are as follows: Q_{1-2} are from W-exchange, Q_{3-6} are from QCD penguin diagrams while Q_{7-10} are from electroweak penguin diagrams.

The energy scale in kaon decays is about 500 MeV, so the hadronic matrix elements of $\mathscr{H}_{eff}$ are dominated by the strong interaction and must be calculated non-perturbatively. The lattice approach is the only possibility for doing this at present, and is currently being used; see Ref.'s [6, 7, 8, 9]. The procedure for calculating the matrix elements from the lattice can be summarized as follows. First one calculates the matrix elements of the appropriate lattice operators $Q_j^{latt}(a)$. Next one matches to the continuum operators at some scale $q^* \approx 1/a$ in a continuum renormalization scheme, *e.g.*, Naive Dimensional Regularization (NDR):

$$Q_i(q^*) = z_{ij}(q^* a) Q_j^{latt}(a) \tag{1.2}$$

The matching factors $z_{ij}(q^* a)$ can be calculated in perturbation theory [12]; they involve $\log(q^* a)$ so the continuum scale q^* must be close to $1/a$ to avoid large logs. Finally, one uses RG evolution to run the continuum operators $Q_i(\mu)$ from the scale $\mu = q^*$ down to $\mu = m_c$ (the charm quark mass) where they can be combined with the known Wilson coefficients[1] at the scale $\mu = m_c$ to get the matrix elements of $\mathscr{H}_{eff}$.[2]

The RG evolution operator required in the final step above has been calculated up to next-to-leading order (NLO) by Buras *et al.* [1]. However, the expression obtained there contains singularities in the case where there are 3 active quark flavors. Therefore it cannot be used for extracting the matrix elements from lattice QCD simulations with $N_f = 2+1$ dynamical fermion flavors. This is a major problem since unquenched lattice simulations with $2+1$ sea quark flavors are currently underway with a variety of fermion discretizations (see, *e.g.*, [10] and references therein) and will be addressing kaon physics such as ε'/ε and the $\Delta I = 1/2$ rule in the coming future. It is therefore imperative to deal with the singularity problem in the NLO expression for the RG evolution operator. The full RG evolution operator is known to be singularity-free, so the singularity in the NLO expression in the 3 flavor case should be a removable artifact. In this paper

[1] The Wilson coefficients are all known up to NLO in peturbation theory [2].

[2] Note that $\mathscr{H}_{eff}$ itself is independent of the scale, so we can combine the operators and Wilson coefficients at any chosen scale to determine its matrix elements.

we review the solution to this problem given recently in Ref.[11]. The singularity is eradicated by a method of analytic continuation to obtain the correct finite NLO expression for the RG operator in the 3 flavor case. Furthermore, we trace the origin of the singularities in the work of Buras *et al.* to a breakdown of their approach in the 3 flavor case, and show how it can be rectified so that singularities are absent from the beginning.

2. Review of RG evolution and the singularity problem at NLO

The running of the $Q_i(\mu)$'s and $C_i(\mu)$'s is governed by the RG evolution equation resulting from $\frac{d}{d\mu}\mathscr{H}_{eff}=0$. Combining the operators and Wilson coefficients into vectors $\vec{Q}$ and $\vec{C}$ respectively, the evolution is given by 10×10 matrices acting on these vectors. The evolution of $\vec{Q}(\mu)$ is obviously inverse to that of $\vec{C}(\mu)$ so it suffices to determine the latter, which is what we do in the following. The running of the EM coupling e is negligible over the range of scales that are relevant for the present considerations, so we treat it as constant in the following, as was done in Ref.[1].

The RG equation for $\vec{C}(\mu)$ is

$$\Big[\mu\frac{\partial}{\partial\mu}+\beta(g,e)\frac{\partial}{\partial g}\Big]\vec{C}=\gamma^T(g,e)\vec{C} \tag{2.1}$$

where $\gamma(g,e)$ is the 10×10 anomalous dimension matrix (given below) and $\beta(g,e)$ is the beta-function, given by

$$\beta(g,e)=-\beta_0\frac{g^3}{16\pi^2}-\beta_1\frac{g^5}{(16\pi^2)^2}-\beta_{1e}\frac{e^2g^3}{(16\pi^2)^2}+\dots \tag{2.2}$$

with

$$\beta_0=11-\frac{2}{3}f\ ,\qquad \beta_1=102-\frac{38}{3}f\ ,\qquad \beta_{1e}=-\frac{8}{9}(u+\frac{d}{4}) \tag{2.3}$$

where u and d denote the number of active $u-$ and $d-$type flavors, respectively, and $f=u+d$ $(=N_f)$ is the total number of active flavors.

From the RG equation (2.1) the running of $\vec{C}(\mu)$ is found to be given by

$$\vec{C}(m_1)=U(m_1,m_2)\vec{C}(m_2) \tag{2.4}$$

where the evolution matrix is

$$U(m_1,m_2)=T_g\exp\Big(\int_{g(m_2)}^{g(m_1)}dg'\,\frac{\gamma^T(g',e)}{\beta(g',e)}\Big) \tag{2.5}$$

with the dependence $g=g(m)$ specified by $m\frac{dg}{dm}=\beta(g,e)$. Here T_g denotes $g-$ordering; it is required since generally $[\gamma(g_1),\gamma(g_2)]\neq 0$ for $g_1\neq g_2$.

To evaluate $U(m_1,m_2)$ we need to know the anomalous dimension matrix $\gamma(g,e)$. It is determined from the renormalization constant matrix relating the bare and renormalized operators: $Q_i^{(0)}=Z_{ij}(\mu)Q_j(\mu)$ and

$$\gamma(g,e)=Z^{-1}\frac{d}{d\log\mu}Z \tag{2.6}$$

This depends on g and e through $\alpha_s = \frac{g^2}{4\pi}$ and $\alpha = \frac{e^2}{4\pi}$, and has been calculated perturbatively up to 2 loops in the NDR scheme, whereby the matrices in the following expansions have been determined (see [1] and the references therein):

$$\gamma(g,e) = \gamma_s(g^2) + \frac{\alpha}{4\pi}\Gamma(g^2) + O(\alpha^2) \tag{2.7}$$

where the pure QCD part is

$$\gamma_s(g^2) = \frac{\alpha_s}{4\pi}\gamma_s^{(0)} + \frac{\alpha_s^2}{(4\pi)^2}\gamma_s^{(1)} + \dots \tag{2.8}$$

and the leading order QED correction in (2.7) is specified by

$$\Gamma(g^2) = \gamma_e^{(0)} + \frac{\alpha_s}{4\pi}\gamma_{se}^{(1)} + \dots \tag{2.9}$$

For later use we note that

$$\begin{aligned} \frac{\gamma(g,e)}{\beta(g,e)} &= -\frac{4\pi}{\beta_0 g^3}\left[\begin{array}{l} \alpha_s\gamma_s^{(0)} + \frac{\alpha_s^2}{4\pi}(\gamma_s^{(1)} - \frac{\beta_1}{\beta_0}\gamma_s^{(0)}) \\ + \alpha\Big(\gamma_e^{(0)} + \frac{\alpha_s}{4\pi}(\gamma_{se}^{(1)} - \frac{\beta_1}{\beta_0}\gamma_e^{(0)} - \frac{\beta_{1e}}{\beta_0}\gamma_s^{(0)}) + O(\alpha_s^2)\Big) + O(\alpha^2) \end{array}\right] && (2.10) \\ &= -\frac{\gamma_s^{(0)}}{\beta_0 g} + O(g) + O(\alpha) && (2.11) \end{aligned}$$

The expansion of the evolution operator in the EM coupling takes the form

$$U(m_1,m_2) = U_s(m_1,m_2) + \frac{\alpha}{4\pi}R(m_1,m_2) + O(\alpha^2) \tag{2.12}$$

where the pure QCD evolution is

$$U_s(m_1,m_2) = T_g \exp\Big(\int_{g(m_2)}^{g(m_1)} dg' \, \frac{\gamma_s^T(g')}{\beta_s(g')}\Big) \tag{2.13}$$

and the leading additional contribution to the QCD evolution in the presence of EM interactions in (2.12) is given by (see [1])

$$R(m_1,m_2) = \int_{g(m_2)}^{g(m_1)} dg' \, \frac{U_s(m_1,m')\Gamma^T(g')U_s(m',m_2)}{\beta_s(g')} \tag{2.14}$$

where $g' = g'(m')$. The EM contribution to the beta-function has been ignored in (2.13)–(2.14): $\beta_s(g) = \beta(g,0)$ so the expressions are valid when the β_{1e} term in (2.2) is dropped, which is a justifiable approximation made in Ref.[1]. However, the generalization of the NLO expressions for the evolution matrix to the case where the β_{1e} term is not dropped is straightforward: In light of (2.10) it can be obtained simply by replacing $\gamma_{se}^{(1)} \to \gamma_{se}^{(1)} - \frac{\beta_{1e}}{\beta_0}\gamma_s^{(0)}$ in the relevant expressions [11].

In the remainder of this paper we restrict our attention to the pure QCD evolution $U_s(m_1,m_2)$ which is where the aforementioned singularity problem arises at NLO in the 3 flavor case. Once the singularity is eradicated, the new finite expression needs to be used in the NLO evaluation of (2.14) for $R(m_1,m_2)$. We omit that part here, referring to Ref.[11] for the details and result.

We begin by recalling the leading logarithmic approximation to $U_s(m_1,m_2)$: it is obtained by keeping only the leading contribution to $\frac{\gamma_s^T(g')}{\beta_s(g')}$ in the integrand in (2.13), which is shown in (2.11). It is useful to diagonalize $\gamma_s^{(0)T}$:

$$\gamma_D^{(0)} = V^{-1}\gamma_s^{(0)T}V \qquad \text{diagonal matrix} \tag{2.15}$$

then the leading logarithmic approximation is found to be

$$U_s^{(0)}(m_1,m_2) = V\Big(\frac{\alpha_s(m_2)}{\alpha_s(m_1)}\Big)^{\gamma_D^{(0)}/2\beta_0}V^{-1} \tag{2.16}$$

The NLO contribution to the evolution matrix can now be found starting from the ansatz

$$U_s(m_1,m_2) = \Big(1+\frac{\alpha_s(m_1)}{4\pi}J\Big)U_s^{(0)}(m_1,m_2)\Big(1-\frac{\alpha_s(m_2)}{4\pi}J\Big) \tag{2.17}$$

and using the RG equation for $U_s(m_1,m_2)$ (given by (2.1) with $\beta(g,e)$ and $\gamma(g,e)$ replaced by $\beta_s(g)$ and $\gamma_s(g)$, respectively) to derive an equation for J. From solving this equation at lowest order in α_s Buras *et al.* find [1, 3]

$$J = VSV^{-1} \tag{2.18}$$

where

$$S_{ij} = \delta_{ij}\gamma_i^{(0)}\frac{\beta_1}{2\beta_0^2} - \frac{G_{ij}}{2\beta_0(1+a_i-a_j)} \tag{2.19}$$

with

$$G = V^{-1}\gamma_s^{(1)}V \quad , \qquad a_i = i\text{'th diagonal element of } \gamma_D^{(0)}/2\beta_0 \tag{2.20}$$

From (2.19) we see that the resulting NLO expression for the evolution matrix has a singularity if $1+a_i-a_j=0$. As mentioned in [1], this happens for $(i,j)=(8,7)$ when there are 3 active quark flavors ($f=3$).

3. Solution of the singularity problem via analytic continuation

The expression (2.17) can be written up to NLO as

$$U_s^{NLO}(m_1,m_2) = U_s^{(0)}(m_1,m_2) + \frac{1}{4\pi}VA(m_1,m_2)V^{-1} \tag{3.1}$$

where

$$VA(m_1,m_2)V^{-1} = \alpha_s(m_1)JU_s^{(0)}(m_1,m_2) - \alpha_s(m_2)U_s^{(0)}(m_1,m_2)J\,. \tag{3.2}$$

Inserting the expression (2.16) for $U_s^{(0)}(m_1,m_2)$ leads to

$$A_{ij}(m_1,m_2) = S_{ij}\Big[\alpha_1\Big(\frac{\alpha_2}{\alpha_1}\Big)^{a_j} - \alpha_2\Big(\frac{\alpha_2}{\alpha_1}\Big)^{a_i}\Big] \tag{3.3}$$

where $\alpha_k \equiv \alpha_s(m_k)$ for $k = 1,2$. In the singular case ($f = 3$, $i = 8$, $j = 7$) we now regularize S_{ij} by replacing

$$a_j \to a_j + \varepsilon \tag{3.4}$$

in (2.19). The regularized quantity then becomes $S_{ij} = \left(\frac{G_{ij}}{2\beta_0}\right)\frac{1}{\varepsilon}$. Inserting this into (3.3), and making the same regularization (3.4) there, we find

$$\begin{aligned} A_{ij}(m_1,m_2) &= \left(\frac{G_{ij}}{2\beta_0}\right)\frac{1}{\varepsilon}\left[\alpha_1\left(\frac{\alpha_2}{\alpha_1}\right)^{a_j+\varepsilon} - \alpha_2\left(\frac{\alpha_2}{\alpha_1}\right)^{a_i}\right] \\ &= \left(\frac{G_{ij}}{2\beta_0}\right)\frac{1}{\varepsilon}\alpha_2\left(\frac{\alpha_2}{\alpha_1}\right)^{a_i}\left[\varepsilon\log\left(\frac{\alpha_2}{\alpha_1}\right) + O(\varepsilon^2)\right] \\ &\overset{\varepsilon\to 0}{=} \left(\frac{G_{ij}}{2\beta_0}\right)\alpha_2\left(\frac{\alpha_2}{\alpha_1}\right)^{a_i}\log\left(\frac{\alpha_2}{\alpha_1}\right) \end{aligned} \tag{3.5}$$

Thus a finite expression is obtained in the limit where the regularization is lifted. Substituting this into (3.1) we get a finite NLO expression for the evolution operator. This solution of the singularity problem clearly amounts to analytic continuation of the evolution operator (regarded as a function of the matrix $\gamma_s^{(0)}$).

4. Understanding the "singularity" from first principles

In the following it is convenient to use the notation $U_s(g_1,g_2)$ rather than $U_s(m_1,m_2)$; this is justified since the dependence on m_1, m_2 enters exclusively through $g(m_1), g(m_2)$.

By general arguments the full evolution operator (for pure QCD) can be written as

$$U_s(g_1,g_2) = \left(1 + \frac{g_1^2}{16\pi^2}J(g_1)\right)U_s^{(0)}(g_1,g_2)\left(1 + \frac{g_2^2}{16\pi^2}J(g_2)\right)^{-1} \tag{4.1}$$

Using the RG equation

$$\frac{d}{dg}U_s(g,g_0) = \frac{\gamma_s^T(g)}{\beta_s(g)}U_s(g,g_0) \tag{4.2}$$

to derive an equation for $J(g)$ at leading order, one finds *different* equations in the "singular" case $1 + a_i - a_j = 0$ and "non-singular" case [11].

In the non-singular case, taking $J(g) = J + O(g)$ leads to a consistent solution for the constant matrix J. This is the solution found by Buras *et al.* that we reviewed in §2. On the other hand, in the singular case, the ansatz $J(g) = J + O(g)$ does *not* admit a consistent solution. In fact, it turns out that $S_{ij}(g) = (V^{-1}J(g)V)_{ij}$ must *diverge* for $g \to 0$. Specifically, in the singular case $1 + a_i - a_j = 0$ we found in Ref.[11] that the leading order equation for $S_{ij}(g)$ is as follows:

$$\beta_0 g\frac{d}{dg}S_{ij}(g) = -G_{ij} \tag{4.3}$$

The solution is

$$S_{ij}(g) = -\frac{G_{ij}}{\beta_0}\log(g) + c_{ij} = -\frac{G_{ij}}{2\beta_0}\log(\alpha_s) + c'_{ij} \tag{4.4}$$

where c_{ij} is an undetermined integration constant and $c'_{ij} = c_{ij} - \frac{G_{ij}}{2\beta_0}\log(4\pi)$. Thus $S_{ij}(g)$ diverges for $g \to 0$ as claimed. Note however that $g^2 S_{ij}(g)$ vanishes for $g \to 0$, implying that $g^2 J(g)$ vanishes in this limit as it should in order for (4.1) to reduce to $U_s^{(0)}(m_1, m_2)$ in the small g limit. We also note that $S_{ij}(g)$ is actually a function of g^2 (or α_s) as it should be. Finally, our previous expression (3.5) for $A_{ij}(m_1, m_2)$ is readily reproduced from (4.4) (see [11]),[3] so the first principles solution of the singularity problem presented here agrees as it should with the finite NLO result for the evolution operator obtained via analytic continuation in the previous section.

5. Conclusions

We have eradicated the singularities in the original solution of Buras *et al.* to get a finite expression for the RG evolution matrix at NLO in the 3 flavor case. This is essential for being able to evaluate the matrix elements of the $\Delta S = 1$ effective Hamiltonian from the lattice with $2+1$ sea quark flavors.

The breakdown of the ansatz $J(g) = J + O(g)$ in Buras *et al.*'s approach, and the rectification discussed here, illustrate some general subtleties to bear in mind when evaluating evolution operators in general.

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