

Before sailing on a domain-wall sea

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ABSTRACT

We discuss the very different roles of the valence-quark and the sea-quark residual masses (m_{res}^v and m_{res}^s) in dynamical domain-wall fermions simulations. Focusing on matrix elements of the effective weak hamiltonian containing a power divergence, we find that m_{res}^v can be a source of a much bigger systematic error. To keep all systematic errors due to residual masses at the 1% level, we estimate that one needs $am_{\text{res}}^s \lesssim 10^{-3}$ and $am_{\text{res}}^v \lesssim 10^{-5}$, at a lattice spacing $a \sim 0.1$ fm. The practical implications are that (1) optimal use of computer resources calls for a mixed scheme with different domain-wall fermion actions for the valence and sea quarks; (2) better domain-wall fermion actions are needed for both the sea and the valence sectors.

1. Introduction

Lattice QCD is entering a stage in which it is becoming more standard to include dynamical fermions (*i.e.* sea quarks) in numerical simulations, in order to move away from the quenched approximation. Needless to say, this step is crucial if lattice QCD is to become really predictive, with full control of all systematic errors.

What has not changed is that simulations with dynamical fermions are very expensive: updating the fermion determinant takes the bulk of the computer time. It is therefore of key importance to choose the parameters of any simulation such that the desired precision of physical observables is obtained. However, in order to use resources wisely, it is equally important to balance the effort with respect to the various systematic errors involved. It is questionable to spend an inordinate amount of computational effort to control one type of error to machine precision, while not controlling some other error to better than, for instance, one percent. This is especially the case if the difference amounts to making the simulation feasible or not.

In the case of domain-wall fermions (DWF) [1, 2], an important systematic error comes from the explicit breaking of chiral symmetry due to the fact that the size of the fifth dimension, L_5 , is kept finite. Chiral symmetry is better at larger L_5 , but the computational cost also grows with L_5 , making the choice of L_5 an optimization problem. Since the cost of simulating the fermion determinant is so large, this optimization problem is particularly acute if one wishes to simulate unquenched lattice QCD using DWF for both the valence- and sea-quark sectors.

In this paper we propose that, given a certain DWF discretization of the Dirac operator, the size of the fifth dimension entering in the sea-quark Dirac operator, L_5^s , may be chosen much smaller than its valence counterpart, L_5^v .¹ This could be of substantial help in reducing the cost of simulations with dynamical DWF, while keeping control over systematic errors due to the lattice-artifact chiral symmetry breaking coming from a finite L_5 .

Since the quality of chiral symmetry is most important in weak hadronic decays, we will center our discussion on the well-known case of non-leptonic kaon decays. In particular, we have in mind the method, proposed long ago [3], of determining physical kaon-decay matrix elements from simpler, unphysical ones, such as $K^+ \rightarrow \pi^+$ and $K^0 \rightarrow 0$, using chiral symmetry. As is well known, power divergences are encountered in this computation, and good chiral symmetry is a key ingredient in controlling it.

We begin with a list of observations, on which this proposal is based. The rest of the paper elaborates on these observations.

Observations

1. Violations of chiral symmetry in Ward–Takahashi (WT) identities and in physical matrix elements arise from the valence sector only, essentially by definition. They vanish when approaching the valence-DWF chiral limit $L_5^v \rightarrow \infty$, in which

¹Superscripts v and s refer to quantities in the valence- and sea-quark sectors, respectively.

the “residual quark mass” (*i.e.* the effective quark mass due to a finite L_5 when the explicit quark mass has been set equal to zero) m_{res}^v goes to zero, regardless of the value of m_{res}^s .

2. Consider any operator \mathcal{Q} belonging to the effective weak hamiltonian, transforming in $(8_L, 1_R)$ of $SU(3)_L \times SU(3)_R$. If $m_{\text{res}}^v = 0$ then, for any m_{res}^s , its power-divergent piece arises from a *single* lower-dimension operator \mathcal{O}_2 . One subtraction, $\mathcal{Q}_{\text{sub}} = \mathcal{Q} - \mathcal{F}\mathcal{O}_2$, defined by the renormalization condition $\langle 0 | \mathcal{Q}_{\text{sub}} | K^0 \rangle = 0$, removes the power divergences from all of its matrix elements simultaneously.
3. We may constrain m_{res}^v and m_{res}^s by the requirement that m_{res} -induced deviations of physical matrix elements from the chiral limit will, for instance, be at the 1% level. Since the systematic effects due to $m_{\text{res}}^v \neq 0$ are magnified by inverse powers of the lattice spacing, we end up with a rather tight constraint on m_{res}^v .
4. Systematic effects due to $m_{\text{res}}^s \neq 0$ alone are *not* magnified by inverse powers of the lattice spacing when following the subtraction procedure defined above. Therefore, chiral perturbation theory gives rise to a milder bound on m_{res}^s . A comparable bound arises from considering m_{res}^s -induced chiral-symmetry violations in the mixing among dimension-six operators as well as scaling violations.

Allowing for m_{res}^s to be much less constrained than m_{res}^v translates into the possibility of choosing L_5^s much smaller than L_5^v . This, in turn, may lead to a substantial economy of computer time, making dynamical DWF simulations possible on currently-planned machines.

The rest of this paper is organized as follows. In Sect. 2, we explain the main observations (1 and 2) in more detail, paying particular attention to power-divergent subtractions. In Sect. 3 we analyze the situation at next-to-leading order (NLO) in chiral perturbation theory (ChPT), with emphasis on the role of $m_{\text{res}}^{v,s}$. As this knowledge will be crucial for the bounds we intend to establish, we give a rather detailed account of the way power divergences relate to low-energy constants (LECs) in ChPT to NLO, including a discussion of short- versus long-distance effects. Sect. 4 then gives estimates of the numerical bounds which $m_{\text{res}}^{v,s}$ need to satisfy in order to determine the leading-order (LO) LECs relevant for $K \rightarrow \pi\pi$ decay to about 1% accuracy, at an inverse lattice spacing of about 2 GeV. In Sect. 5 we discuss the implications of our results. The systematics of residual chiral symmetry violating effects is discussed in Appendix A.

2. Power divergences

2.1 Setup and (chiral) symmetry considerations (Observation 1)

It is easiest to illustrate the very different roles of the sea and valence chiral symmetries in a simplified, extreme case where the valence quarks have an exact chiral

symmetry (for $m_q^v = 0$), while the sea quarks are Wilson fermions, with basically no chiral symmetry at finite lattice spacing. This “mixed” framework was studied recently in a chiral-lagrangian framework in ref. [4].

We will assume the number of valence quarks to be N_v , and the number of sea quarks to be N_s . With a mixed action, there is no (exact) symmetry that mixes the valence and sea quarks. With Wilson sea quarks and Ginsparg–Wilson valence (and ghost) quarks, the lattice flavor symmetries are

$$\begin{aligned} G_{sea} &= U(N_s)_V \\ G_{val} &= [SU(N_v|N_v)_L \otimes SU(N_v|N_v)_R] \circledast U(1)_V. \end{aligned} \quad (2.1)$$

The \circledast symbol denotes a semi-direct product.

Let us now consider an axial WT identity. It is obtained by applying a (local) axial transformation to the valence quarks *only* (and not to either sea or ghost quarks). Since the (global) non-singlet axial symmetry of the valence quarks is exact, there are no lattice-artifact chiral symmetry violating terms in the resulting WT identity. This is true in particular for the PCAC relation, implying that the (valence-quark) pion mass must vanish exactly for $m_v = 0$. Whether or not the sea quarks have an axial symmetry plays no role here! All that is necessary is that the gauge fields do not transform under the flavor symmetries, and therefore there is no way to “communicate” (axial) flavor transformations applied to valence quarks to the sea quarks.

2.2 Application to $K \rightarrow \pi$ penguins (Observation 2)

Similar considerations apply to any operator mixing which occurs in the calculation of physical matrix elements. The basic reason is that, by definition, the operators that interpolate the external states are made of valence quarks only. This can be best illustrated through an example.

In the calculation of matrix elements needed for $K \rightarrow \pi\pi$, the most dangerous mixings are the power-divergent subtractions. This allows the four-fermion operators occurring in those matrix elements to mix with the fermion bilinear [3]

$$\begin{aligned} \mathcal{O}_2 &= \bar{s}\gamma_\mu(\vec{D}_\mu - \overleftarrow{D}_\mu)(1 - \gamma_5)d \\ &\stackrel{\circ}{=} (m_s + m_d)\bar{s}d + (m_d - m_s)\bar{s}\gamma_5d, \end{aligned} \quad (2.2)$$

where $\stackrel{\circ}{=}$ denotes on-shell equality.² In full continuum QCD the operators that can mix with a fermion bilinear are the $(8_L, 1_R)$ ones. In a hybrid scheme, the four-fermion operator must contain valence \bar{s} and d . The other two fermions may be valence, sea, or ghost quarks. When the valence sector has the exact chiral symmetry of Eq. (2.1) with $N_v = 3$, the effective weak hamiltonian contains four-fermion operators which transform as $(8_L, 1_R)$ under $SU(3)_L \times SU(3)_R \subset G_{val}$. They can thus mix with an $\bar{s}d$ bilinear with the same quantum numbers (including *CPS* symmetry [3], under which

²In this paper, we only consider matrix elements with on-shell external states, and we may thus use the equations of motion. However, we will allow for matrix elements which do not conserve momentum.

the weak hamiltonian is even).³ In order to be able to use the G_{val} symmetry in constructing such bilinears, the quark mass matrix M is promoted to a spurion field, transforming as $M \rightarrow LMR^\dagger$, with $L, R \in SU(N_v|N_v)_{L,R}$. The only fermion bilinear with dimension smaller than six satisfying these requirements is \mathcal{O}_2 . This operator has mass-dimension four, and hence it mixes with the octet weak hamiltonian through a coefficient proportional to $1/a^2$. It also follows that there is no mixing of order $1/a$, because a dimension-five operator with the appropriate quantum numbers does not exist.

2.3 Renormalization condition for the power divergence

In field theory one renormalizes operators, not individual matrix elements.⁴ Given a four-fermion operator \mathcal{Q} which mixes with \mathcal{O}_2 , we thus need to define a subtracted operator

$$\mathcal{Q}_{\text{sub}} = \mathcal{Q} - \mathcal{F} \mathcal{O}_2. \quad (2.3)$$

Here \mathcal{F} is a dimensionful function of the parameters of the theory which diverges like $1/a^2$. Among these parameters are the explicit quark masses contained in the lattice action. If we assign to the mass parameters their spurion transformation properties, \mathcal{F} must be invariant under all symmetries (for the hybrid theory, this includes in particular the symmetries of Eq. (2.1) and CPS).

As already mentioned, no lower-dimension operator other than \mathcal{O}_2 has the quantum numbers of \mathcal{Q} . (This is not true if $m_{\text{res}}^v \neq 0$, see below.) Hence, a single renormalization condition is sufficient to determine the subtraction. Moreover, the single subtraction (2.3) must remove the entire power-divergent part of \mathcal{Q} (see below for logarithmic divergences). Here we choose the homogeneous renormalization condition⁵

$$0 = \langle 0 | \mathcal{Q}_{\text{sub}} | K^0 \rangle = \langle 0 | \mathcal{Q} | K^0 \rangle - \mathcal{F} (m_d - m_s) \langle 0 | \bar{s} \gamma_5 d | K^0 \rangle, \quad (2.4)$$

which yields

$$\mathcal{F} = \frac{\langle 0 | \mathcal{Q} | K^0 \rangle}{(m_d - m_s) \langle 0 | \bar{s} \gamma_5 d | K^0 \rangle}. \quad (2.5)$$

Equation (2.4) is a consistent renormalization condition because, for $m_d \neq m_s$, the power-divergent part of \mathcal{Q} contributes to the matrix element at LO in ChPT. Indeed, the power divergence corresponds to (the matrix element of) the operator $\bar{s} \gamma_5 d$. This operator is a total divergence on shell, which contributes to $K^0 \rightarrow 0$ because momentum is not conserved in that matrix element [3]. Since momentum is conserved for the physical $K \rightarrow \pi\pi$ matrix elements, one does have that $\langle \pi\pi | \mathcal{O}_2 | K \rangle = 0$.

Before we move on, we need to discuss the freedom in choosing the renormalization condition. Generically, a physical renormalization condition may be written

³In the case of the strong penguins $Q_{5,6}$ only the ‘‘partially-quenched singlet (PQS)’’ operators of ref. [5] can mix with $\bar{s}d$. In this paper, we consider only PQS operators.

⁴For a similar discussion in this context, see Ref. [6].

⁵This renormalization condition was also discussed in the context of the direct determination of $K \rightarrow \pi\pi$ matrix elements in ref. [7].

as $\langle A | \mathcal{Q}_{\text{sub}} | B \rangle = C$, where $|A\rangle$ and $|B\rangle$ are some states, and the (not necessarily zero) constant C is finite in physical units. How does changing the renormalization condition affect the subtracted operator and its matrix elements? Let us expand the subtraction coefficient in Eq. (2.3) as a power series in a :

$$\mathcal{F}(a) = \frac{\mathcal{F}_2}{a^2} + \mathcal{F}_0 + O(a). \quad (2.6)$$

If we choose a different renormalization condition, we will end up with a new subtraction coefficient

$$\mathcal{F}'(a) = \frac{\mathcal{F}'_2}{a^2} + \mathcal{F}'_0 + O(a). \quad (2.7)$$

How are $\mathcal{F}(a)$ and $\mathcal{F}'(a)$ related? Let $\mathcal{Q}'_{\text{sub}} = \mathcal{Q} - \mathcal{F}'\mathcal{O}_2$. Then

$$\begin{aligned} \langle 0 | \mathcal{Q}'_{\text{sub}} | K^0 \rangle &= \langle 0 | \mathcal{Q} | K^0 \rangle - \left(\frac{\mathcal{F}'_2}{a^2} + \mathcal{F}'_0 + O(a) \right) (m_d - m_s) \langle 0 | \bar{s} \gamma_5 d | K^0 \rangle \\ &= \left(\frac{\mathcal{F}_2 - \mathcal{F}'_2}{a^2} + \mathcal{F}_0 - \mathcal{F}'_0 + O(a) \right) (m_d - m_s) \langle 0 | \bar{s} \gamma_5 d | K^0 \rangle. \end{aligned} \quad (2.8)$$

The last equality is true because $\langle 0 | \mathcal{Q}_{\text{sub}} | K^0 \rangle = 0$ by construction. We see that $\langle 0 | \mathcal{Q}'_{\text{sub}} | K^0 \rangle$ is finite *if and only if* $\mathcal{F}_2 = \mathcal{F}'_2$. Now, since \mathcal{Q} can mix with only one lower-dimension operator, it follows that any consistent renormalization condition must give rise to the same value for \mathcal{F}_2 . In other words, the power-divergent part of \mathcal{F} is *independent* of the renormalization condition, but the finite part is not. (That is, in general $\mathcal{F}_0 \neq \mathcal{F}'_0$. Of course, the same is true for the $O(a)$ part.) In the case at hand, the subtraction defined by Eq. (2.3) and the renormalization condition $\langle 0 | \mathcal{Q}_{\text{sub}} | K^0 \rangle = 0$ ensures the absence of power divergences in $\langle \pi | \mathcal{Q}_{\text{sub}} | K \rangle$ and $\langle \pi \pi | \mathcal{Q}_{\text{sub}} | K \rangle$ simultaneously. Denoting the coefficient of $1/a^2$ in the divergent part of a matrix element by “*div*,” this statement can be summarized in the suggestive form

$$\frac{\text{div} \langle A | \mathcal{Q} | B \rangle}{\langle A | \mathcal{O}_2 | B \rangle} = \frac{\text{div} \langle 0 | \mathcal{Q} | K^0 \rangle}{\langle 0 | \mathcal{O}_2 | K^0 \rangle} = \mathcal{F}_2, \quad (2.9)$$

for any two states $\langle A |$ and $| B \rangle$.

The matrix elements of \mathcal{Q}_{sub} will in general still contain logarithmic divergences. Fully renormalized operators may be defined on the lattice using *e.g.* the regularization independent (RI) non-perturbative renormalization (NPR) method [8, 6]. (For a different method, see ref. [9].) Renormalized operators $\mathcal{Q}_r^i = \mathcal{Z}_j^i \mathcal{Q}_{\text{sub}}^j$ are defined by the requirement that their matrix element between given (gauge fixed, off shell) high-momentum four-quark states has a prescribed value. Typically, one performs a second (finite) renormalization in order to relate the lattice-renormalized operators to renormalized operators defined in some continuum scheme such as $\overline{\text{MS}}$.

The entire renormalization procedure discussed above does not rely on the effective chiral lagrangian. The numerical extraction of \mathcal{F}^j can be done directly from Eq. (2.4). Similarly, the NPR matrix \mathcal{Z}_j^i is determined numerically. In the case at hand, we obtain renormalized $K \rightarrow \pi$ matrix elements (ignoring for simplicity the renormalization of the external states) via

$$\langle \pi | \mathcal{Q}_r^i | K \rangle = \mathcal{Z}_j^i \langle \pi | \mathcal{Q}_{\text{sub}}^j | K \rangle = \mathcal{Z}_j^i \left(\langle \pi | \mathcal{Q}^j | K \rangle - \mathcal{F}^j (m_d + m_s) \langle \pi | \bar{s} d | K \rangle \right). \quad (2.10)$$

This result can now be matched on to the appropriate ChPT expression. The LECs obtained this way are then used to determine the $K \rightarrow \pi\pi$ matrix elements.

While it is clear that the complete renormalization is carried out without using ChPT, the ChPT calculation must conform to the actual renormalization procedure that we envisage performing numerically. We will return to this point below.

3. Chiral perturbation theory

In this section we work out a ChPT example. The central point is that, as long as $m_{\text{res}}^v = 0$, the above procedure completely removes the power-divergences even if both the un-subtracted \mathcal{Q} and \mathcal{O}_2 matrix elements depend on m_{res}^s .

3.1 Matrix elements of \mathcal{Q} and \mathcal{O}_2 for $m_{\text{res}} = 0$

We begin with the representation of a general weak $(8_L, 1_R)$ operator to NLO in ChPT in the continuum, working in the limit in which $m_{\text{res}}^{v,s} = 0$. In this case, the theory is partially quenched [10], with an enlarged symmetry group⁶

$$[SU(N_v + N_s|N_v)_L \times SU(N_v + N_s|N_v)_R] \times U(1)_V. \quad (3.1)$$

Any octet operator \mathcal{Q} mediating $\Delta S = 1$ transitions can be written as (in euclidean space)⁷

$$\begin{aligned} \mathcal{Q} &= \mathcal{Q}_2 + \mathcal{Q}_4 + \dots, \\ \mathcal{Q}_2 &= -\alpha_1^8 \text{str}(\Lambda L_\mu L_\mu) + \alpha_2^8 \text{str}(\Lambda X_+), \\ \mathcal{Q}_4 &= \frac{1}{(4\pi f)^2} \left(\sum_i \beta_i^8 \mathcal{O}_i^8 + \sum_i \tilde{\beta}_i^8 \tilde{\mathcal{O}}_i^8 \right), \end{aligned} \quad (3.2)$$

in which α_i^8 and β_i^8 denote LECs at LO and NLO, respectively, and

$$\Lambda_j^i = \delta_{i3} \delta_{j2}. \quad (3.3)$$

In terms of the non-linear field $\Sigma = \exp(2i\Phi/f)$,

$$\begin{aligned} L_\mu &= i\Sigma \partial_\mu \Sigma^\dagger, \\ X_\pm &= 2B_0(\Sigma M^\dagger \pm M \Sigma^\dagger). \end{aligned} \quad (3.4)$$

M is the (diagonal) quark mass matrix containing the valence, sea and ghost quark masses and, after promotion to a spurion field, transforming just like Σ under the full chiral group $G_L \times G_R$, $\Sigma \rightarrow L \Sigma R^\dagger$, with $L, R \in G_{L,R}$. The list of NLO operators relevant for our purposes is [13]

$$\mathcal{O}_1^8 = \text{str}(\Lambda X_+ X_+), \quad (3.5)$$

⁶For our purposes, it is sufficient to consider this symmetry group, even though the actual symmetry group is slightly different, see Refs. [11].

⁷We will use the notations and conventions of ref. [12].

$$\begin{aligned}
\mathcal{O}_2^8 &= \text{str}(\Lambda X_+) \text{str}(X_+), \\
\mathcal{O}_3^8 &= \text{str}(\Lambda X_- X_-), \\
\mathcal{O}_4^8 &= \text{str}(\Lambda X_-) \text{str}(X_-), \\
\mathcal{O}_5^8 &= \text{str}(\Lambda [X_+, X_-]), \\
\mathcal{O}_{10}^8 &= \text{str}(\Lambda \{X_+, L_\mu L_\mu\}), \\
\mathcal{O}_{11}^8 &= \text{str}(\Lambda L_\mu X_+ L_\mu), \\
\mathcal{O}_{13}^8 &= \text{str}(\Lambda X_+) \text{str}(L_\mu L_\mu), \\
\mathcal{O}_{14}^8 &= \text{str}(\Lambda L_\mu L_\mu) \text{str}(X_+), \\
\mathcal{O}_{15}^8 &= \text{str}(\Lambda [X_-, L_\mu L_\mu]).
\end{aligned}$$

There are two total-derivative operators relevant for our discussion [12],

$$\tilde{\mathcal{O}}_1^8 = i\partial_\mu \text{str}(\Lambda [L_\mu, X_+]), \quad \tilde{\mathcal{O}}_2^8 = i\partial_\mu \text{str}(\Lambda \{L_\mu, X_-\}). \quad (3.6)$$

In partially quenched QCD, \mathcal{O}_{14}^8 is an independent operator, which cannot be written in terms of the other operators [14].⁸ However, the operators \mathcal{O}_1^8 , \mathcal{O}_3^8 and \mathcal{O}_5^8 are not independent:

$$\mathcal{O}_1^8 - \mathcal{O}_3^8 + \mathcal{O}_5^8 = 4 \text{str}(\Lambda M M^\dagger) = 0, \quad (3.7)$$

where the latter equality holds because M is diagonal. Henceforth, we will set $\beta_5^8 = 0$.

We also need the ChPT representation of the operator \mathcal{O}_2 to NLO. This operator can be written as the $\Delta S = 1$ part of the variation of the (continuum) QCD lagrangian under a chiral rotation which transforms $M \rightarrow (\Lambda + \Lambda^\dagger)M$. Since the QCD lagrangian is represented in ChPT by the strong chiral lagrangian, all we need to do is to perform this same chiral rotation on the strong chiral lagrangian. Doing this, keeping only the Λ ($\Delta S = +1$) part, one obtains [13]

$$\begin{aligned}
\mathcal{O}_2 &= \frac{f^2}{8} \text{str}(\Lambda X_+) \\
&+ (L_8 + \frac{1}{2}H_2)\mathcal{O}_1^8 + 2L_6\mathcal{O}_2^8 + (L_8 - \frac{1}{2}H_2)\mathcal{O}_3^8 + 2L_7\mathcal{O}_4^8 + \frac{1}{2}H_2\mathcal{O}_5^8 \\
&+ \frac{1}{2}L_5\mathcal{O}_{10}^8 + L_4\mathcal{O}_{13}^8 - \frac{1}{2}L_5\mathcal{O}_{15}^8 + \tilde{L}_1(\tilde{\mathcal{O}}_1^8 + \tilde{\mathcal{O}}_2^8),
\end{aligned} \quad (3.8)$$

where L_i and H_2 are $O(p^4)$ Gasser–Leutwyler coefficients [15]; $\tilde{\mathcal{O}}_1^8 + \tilde{\mathcal{O}}_2^8$ is the chiral rotation of $2i\partial_\mu \text{str}(L_\mu X_-)$, and \tilde{L}_1 is a new strong LEC multiplying this operator. We have added this total-derivative operator just as we did in Eq. (3.2). (The operator \mathcal{O}_2 is a local operator, not integrated over space-time. So, more precisely, one may obtain the operator \mathcal{O}_2 by doing the chiral rotation on the strong energy-momentum tensor, which may contain total-derivative terms.) We may set $H_2 = 0$ because of Eq. (3.7).

It is now straightforward to calculate \mathcal{F} , defined in Eq. (2.5), to NLO in ChPT, using the results for $\langle 0 | \mathcal{Q} | K^0 \rangle$ from ref. [12], and Eq. (3.8) above. Since at LO only

⁸A point which has been overlooked in ref. [12].

$\text{str}(\Lambda X_+)$ contributes to $K^0 \rightarrow 0$, the chiral logarithms proportional to α_2^8 drop out of \mathcal{F} , and we find

$$\begin{aligned} \mathcal{F} &= \frac{8}{f^2} \left[\alpha_2^8 + \alpha_1^8 \times (\text{chiral logs}) \right. \\ &\quad \left. + \frac{B_0}{(4\pi f)^2} \left((4\beta_1^8 - 32\lambda_8\alpha_2^8 + 2\tilde{\beta}_1^8 - 16\tilde{\lambda}_1^8\alpha_2^8)(m_s + m_d) + (4\beta_2^8 - 64\lambda_6\alpha_2^8) \sum_i m_i^s \right) \right], \end{aligned} \quad (3.9)$$

in which

$$\lambda_i = 16\pi^2 L_i. \quad (3.10)$$

We may now use this result for \mathcal{F} to define the subtracted operator \mathcal{Q}_{sub} in ChPT, and calculate its $K^+ \rightarrow \pi^+$ matrix element for degenerate valence quark masses m^v . We find that the LO terms proportional to α_2^8 , as well as the chiral logarithms generated at NLO by the corresponding operators, cancel in the matrix elements $\langle \pi^+ | \mathcal{Q} | K^+ \rangle$ and $\mathcal{F} \langle \pi^+ | \mathcal{O}_2 | K^+ \rangle$, leaving us with the result

$$\begin{aligned} \langle \pi^+ | \mathcal{Q}_{\text{sub}} | K^+ \rangle &= \frac{8B_0 m^v}{f^2} \left[\alpha_1^8 (1 + \text{chiral logs}) \right. \\ &\quad - \frac{4B_0}{(4\pi f)^2} \left((2\beta_3^8 + 2\beta_{10}^8 + \beta_{11}^8 + 8\lambda_5(\alpha_1^8 - \alpha_2^8) - 16\lambda_8(\alpha_1^8 + \alpha_2^8) - \tilde{\beta}_1^8 + 8\tilde{\lambda}_1^8\alpha_2^8) m^v \right. \\ &\quad \left. \left. + (\beta_{14}^8 - 16\lambda_6\alpha_1^8 + 8\lambda_4\alpha_1^8) \sum_i m_i^s \right) \right], \end{aligned} \quad (3.11)$$

where we took the limit $m_s \rightarrow m_d = m^v$ in expression (3.9) for \mathcal{F} .

The ‘‘chiral logs’’ are those coming from the α_1^8 operator in Eq. (3.2), and an explicit expression can be found in ref. [12].⁹ The NLO terms proportional to α_1^8 come from the fact that we expressed the common mass M_{phys} of the physical (valence) meson, which appears at LO in the α_1^8 term, in terms of the valence quark mass m^v and the sea quark masses m_i^s , using

$$(M_{phys})^2 = 2B_0 m^v \left(1 + \text{chiral logs} + \frac{32B_0}{(4\pi f)^2} \left[(2\lambda_8 - \lambda_5)m^v + (2\lambda_6 - \lambda_4) \sum_i m_i^s \right] \right). \quad (3.12)$$

Finally, we omitted wave-function renormalizations for the states $|K^+\rangle$ and $|\pi^+\rangle$.

Let us discuss what we learn from these results. In the NLO part of Eq. (3.11), m^v and $\sum_i m_i^s$ are multiplied by linear combinations of LECs having the generic form

$$\sum_i c_i \beta_i^8 - \alpha_2^8 \sum_j d_j \lambda_j, \quad (3.13)$$

where c_i and d_j are numerical coefficients. We know from the general arguments of Sect. 2 that the subtracted matrix element in Eq. (3.11) contains no power divergence. Since m^v and m_i^s are free parameters, it follows that the linear combinations (3.13) are not power divergent either! This simple observation leads to several important conclusions.

⁹See Eq. (4.19) of that paper.

Corollary 1. Some of the LECs β_i^8 diverge like $1/a^2$, just like α_2^8 . *Proof:* The linear combination $\sum_j d_j \lambda_j$ occurring in expression (3.13) will in general be non-zero. Since α_2^8 diverges like $1/a^2$, so must $\sum_i c_i \beta_i$. (This observation is implicit in the work of ref. [14].)

Corollary 2. At NLO, un-subtracted matrix elements contain contributions that diverge like $(1/a^2)(B_0 m/f^2)^n$ for both $n = 1$ and $n = 2$. (Here m stands for a generic mass parameter.) *Proof:* For $n = 1$ this is evident from the LO result. For $n = 2$, observe that whenever \mathcal{O}_i^8 occurs in the matrix element $\langle \pi^+ | \mathcal{O}_2 | K^+ \rangle$ with a non-zero coefficient, the corresponding (power divergent!) LEC β_i^8 occurs in $\langle \pi^+ | \mathcal{Q} | K^+ \rangle$, where it is multiplied by $(B_0 m/f^2)^2$. It is quite evident that, as we go to higher orders in ChPT, un-subtracted matrix elements will contain divergent pieces $(1/a^2)(B_0 m/f^2)^n$ with correspondingly higher values of n .

The last observation may seem surprising at first, because intuitively one expects that short-distance divergences should be insensitive to long-distance effects. We believe that this intuitive notion is, in fact, correct, but it has to be stated more carefully. This leads us to the following two conjectures.

Conjecture 1. For any operator \mathcal{O}_i^8 occurring in the NLO representation of \mathcal{O}_2 , the linear combination $\beta_i^{\text{sub}} = \beta_i - 8\alpha_2^8 \sum_j e_{ij} \lambda_j$ contains no power divergence. Here the linear combination $\sum_j e_{ij} \lambda_j$ is equal to the combination of strong LECs that multiplies \mathcal{O}_i^8 in Eq. (3.8),¹⁰ with $L_j \rightarrow \lambda_j$.¹¹

It is easy to understand why the combinations β_i^{sub} should be finite. Seven of the NLO operators \mathcal{O}_i^8 in Eq. (3.5) as well as the two total-derivative operators in Eq. (3.6) occur in the representation of \mathcal{O}_2 (Eq. (3.8)). Separately, the matrix elements $\langle A | \mathcal{Q} | B \rangle$ and $\mathcal{F} \langle A | \mathcal{O}_2 | B \rangle$ each diverge like $1/a^2$. But taken together they yield $\langle A | \mathcal{Q}_{\text{sub}} | B \rangle$, which must be finite. If we now consider a sufficiently large collection of matrix elements (corresponding to various choices of $\langle A |$ and/or $| B \rangle$), we expect that, for each i , $\langle A | \mathcal{O}_i^8 | B \rangle$ will depend in a different way on all the quark masses. The obvious way for all the subtracted matrix elements to be finite simultaneously is, therefore, that the β_i^{sub} be finite. As an example of this, the combinations β_{14}^8 and $2(\beta_3^8 - 8\lambda_8 \alpha_2^8) + 2(\beta_{10}^8 - 4\lambda_5 \alpha_2^8) + \beta_{11}^8 - (\tilde{\beta}_1^8 - 8\lambda_1 \alpha_2^8)$ in Eq. (3.11) have to be finite. We thus believe that it is only a matter of more work to prove that all the β_i^{sub} 's are in fact finite.

Our next conjecture deals with the separation of short- and long-distance effects.

Conjecture 2. The subtraction coefficient \mathcal{F} defined in Eq. (2.4) contains no divergences of the form $(1/a^2)(B_0 m/f^2)^n$ for $n \geq 1$. In other words, \mathcal{F}_2 (Eq. (2.6)) corresponds only to the α_2^8 term in Eq. (3.9) and is independent of all mass parameters, while the finite \mathcal{F}_0 corresponds to the entire NLO part of Eq. (3.9).

The evidence supporting this conjecture is that the NLO part of \mathcal{F} , Eq. (3.9), can be expressed as a function of β_i^{sub} only. Conjecture 2 thus follows from Conjecture 1, to NLO. We believe that this demonstrates in the case at hand how the short-distance

¹⁰By inspection, for each i , e_{ij} is non-zero only for one value of j .

¹¹This claim is already contained in ref. [14], see in particular Table 5 therein.

divergences are disentangled from the long-distance physics.

In matrix elements, the short-distance divergences get multiplied by factors that originate from the long-distance physics of the matrix element. It should therefore come as no surprise that *un-subtracted* matrix elements contain divergences of the form $(1/a^2)(B_0 m/f^2)^n$ for $n \geq 1$.

Our results for \mathcal{F} and $\langle \pi^+ | \mathcal{O}_{\text{sub}} | K^+ \rangle$ are different from those found in ref. [14].¹² The reason is that in ref. [14] the subtraction condition Eq. (2.4) was only imposed to LO in ChPT, taking $\mathcal{F} = 8\alpha_2^8/f^2$ instead of Eq. (3.9). This amounts to using a different subtraction condition, because the NLO combinations $\beta_1^8 - 8\lambda_8\alpha_2^8$, $\tilde{\beta}_1^8 - 8\tilde{\lambda}_1^8\alpha_2^8$ and $\beta_2^8 - 16\lambda_6\alpha_2^8$ are finite (up to logarithms), as we argued above. Thus, to NLO, the subtraction condition used in ref. [14] is of the form $\langle 0 | \mathcal{Q}'_{\text{sub}} | K^0 \rangle = C \neq 0$, with C finite. Comparing to Eq. (2.8), indeed $\mathcal{F}_2 = \mathcal{F}'_2$, but $\mathcal{F}_0 - \mathcal{F}'_0$ does not vanish, and is given by the NLO terms of Eq. (3.9).

While both subtraction conditions thus remove power divergences from all matrix elements, the subtraction condition of Eq. (2.4) is easier to implement numerically, because no reference to ChPT is made. The condition discussed in ref. [14] distinguishes between LO and NLO, and therefore its implementation requires fitting to the appropriate ChPT expressions.

Finally, we emphasize again that physical results do not depend on which subtraction condition is chosen, because $\langle \pi^+\pi^- | \mathcal{O}_2 | K^0 \rangle = 0$. As already mentioned, at the level of quark operators, this equality follows from the fact that the parity-odd part of \mathcal{O}_2 is a total divergence on-shell; this argument can be carried over to ChPT using the chiral WT identities.

3.2 The case $m_{\text{res}} \neq 0$

We now investigate how the situation changes when $m_{\text{res}} \neq 0$. The chiral symmetry breaking, present in lattice QCD with domain-wall fermions due to the fact that the limit $L_5 \rightarrow \infty$ is not taken, can be represented by a local operator transforming in the same way as an explicit mass term [2]. We take the effect of this chiral symmetry breaking into account by introducing a new spurion field M_{res} , which is then set equal to

$$M_{\text{res}} = \text{diag}(m_{\text{res}}^v, \dots, m_{\text{res}}^s, \dots, m_{\text{res}}^v, \dots). \quad (3.14)$$

M_{res} is expected to be small if both valence and sea quarks are well outside the Aoki phase [17]. The first and last set of entries refer to the valence and ghost sectors, while the middle set of entries refers to the sea sector. Both m_{res}^v and m_{res}^s are flavor independent. (For a more detailed discussion of the systematics of residual chiral symmetry violations, see Appendix A.) We may thus define new building blocks for operators in the effective theory [16]:

$$X_{\pm}^{\text{res}} = 2B_0(\Sigma M_{\text{res}}^{\dagger} \pm M_{\text{res}} \Sigma^{\dagger}). \quad (3.15)$$

The choice of $2B_0$ as a proportionality factor defines the normalization of $m_{\text{res}}^{v,s}$.

¹²See Eq. (62) of that paper.

The presence of M_{res} leads to new *CPS*-even operators in the effective theory:

$$\begin{aligned}
\alpha_2^8 \text{str}(\Lambda X_+) &\rightarrow \theta_2 \text{str}(\Lambda X_+^{\text{res}}), & (3.16) \\
\beta_1^8 \mathcal{O}_1^8 &\rightarrow \eta_{1,1} \text{str}(\Lambda \{X_+, X_+^{\text{res}}\}) + \eta_{1,2} \text{str}(\Lambda X_+^{\text{res}} X_+^{\text{res}}), \\
\beta_2^8 \mathcal{O}_2^8 &\rightarrow \eta_{2,1} \text{str}(\Lambda X_+) \text{str}(X_+^{\text{res}}) + \eta_{2,2} \text{str}(\Lambda X_+^{\text{res}}) \text{str}(X_+) \\
&\quad + \eta_{2,3} \text{str}(\Lambda X_+^{\text{res}}) \text{str}(X_+^{\text{res}}), \\
\beta_3^8 \mathcal{O}_3^8 &\rightarrow \eta_{3,1} \text{str}(\Lambda \{X_-, X_-^{\text{res}}\}) + \eta_{3,2} \text{str}(\Lambda X_-^{\text{res}} X_-^{\text{res}}), \\
\beta_4^8 \mathcal{O}_4^8 &\rightarrow \eta_{4,1} \text{str}(\Lambda X_-) \text{str}(X_-^{\text{res}}) + \eta_{4,2} \text{str}(\Lambda X_-^{\text{res}}) \text{str}(X_-) \\
&\quad + \eta_{4,3} \text{str}(\Lambda X_-^{\text{res}}) \text{str}(X_-^{\text{res}}), \\
\beta_{10}^8 \mathcal{O}_{10}^8 &\rightarrow \eta_{10} \text{str}(\Lambda \{X_+^{\text{res}}, L_\mu L_\mu\}), \\
\beta_{11}^8 \mathcal{O}_{11}^8 &\rightarrow \eta_{11} \text{str}(\Lambda L_\mu X_+^{\text{res}} L_\mu), \\
\beta_{13}^8 \mathcal{O}_{13}^8 &\rightarrow \eta_{13} \text{str}(\Lambda X_+^{\text{res}}) \text{str}(L_\mu L_\mu), \\
\beta_{14}^8 \mathcal{O}_{14}^8 &\rightarrow \eta_{14} \text{str}(\Lambda L_\mu L_\mu) \text{str}(X_+^{\text{res}}), \\
\beta_{15}^8 \mathcal{O}_{15}^8 &\rightarrow \eta_{15} \text{str}(\Lambda [X_-^{\text{res}}, L_\mu L_\mu]).
\end{aligned}$$

In the strong effective lagrangian, there are new LO and NLO operators of the form (giving only the ones relevant for the matrix elements of interest)

$$\begin{aligned}
\text{str}(X_+) &\rightarrow \text{str}(X_+^{\text{res}}), & (3.17) \\
\lambda_4 \text{str}(L_\mu L_\mu) \text{str}(X_+) &\rightarrow \kappa_4 \text{str}(L_\mu L_\mu) \text{str}(X_+^{\text{res}}), \\
\lambda_5 \text{str}(L_\mu L_\mu X_+) &\rightarrow \kappa_5 \text{str}(L_\mu L_\mu X_+^{\text{res}}), \\
\lambda_6 (\text{str} X_+)^2 &\rightarrow \kappa_{6,1} \text{str}(X_+) \text{str}(X_+^{\text{res}}) + \kappa_{6,2} (\text{str} X_+^{\text{res}})^2, \\
\lambda_7 (\text{str} X_-)^2 &\rightarrow \kappa_{7,1} \text{str}(X_-) \text{str}(X_-^{\text{res}}) + \kappa_{7,2} (\text{str} X_-^{\text{res}})^2, \\
\lambda_8 \text{str}(X_+^2 + X_-^2) &\rightarrow \kappa_{8,1} \text{str}(X_+ X_+^{\text{res}} + X_- X_-^{\text{res}}) + \kappa_{8,2} \text{str}((X_+^{\text{res}})^2 + (X_-^{\text{res}})^2).
\end{aligned}$$

The contributions of these new operators to \mathcal{O}_2 can easily be obtained by applying the chiral rotation $M \rightarrow (\Lambda + \Lambda^\dagger)M$, $M_{\text{res}} \rightarrow (\Lambda + \Lambda^\dagger)M_{\text{res}}$ to these new operators.

First consider the case that only $m_{\text{res}}^s \neq 0$, while $m_{\text{res}}^v = 0$, *i.e.* the valence quarks have the same chiral symmetry as in the continuum theory. Clearly, for fixed, non-zero m_{res}^s , the symmetry group of Eq. (3.1) gets broken to the group of Eq. (2.1). Keeping only tree-level contributions from both LO operators and from the NLO operators listed in Eq. (3.16), we find that

$$\langle 0|Q|K^0\rangle = \frac{4iB_0(m_s - m_d)}{f} \left(\alpha_2^8 + \frac{4B_0}{(4\pi f)^2} \eta_{2,1} N_s m_{\text{res}}^s \right), \quad (3.18)$$

$$\langle \pi^+|Q|K^+\rangle = \frac{8B_0 m^v}{f^2} \left(\alpha_1^8 - \frac{4B_0}{(4\pi f)^2} \eta_{14} N_s m_{\text{res}}^s - \left(\alpha_2^8 + \frac{4B_0}{(4\pi f)^2} \eta_{2,1} N_s m_{\text{res}}^s \right) \right), \quad (3.19)$$

in which m^v is again the degenerate valence quark mass in the $K^+ \rightarrow \pi^+$ decay.¹³ One

¹³We see that all that happens is that, in the un-subtracted matrix elements, the LECs α_1^8 and α_2^8 “get shifted” by an amount proportional to m_{res}^s . This is a natural consequence of the form of the relevant NLO operators. The reader can verify that any “shift” in α_2^8 drops out of the subtracted matrix element.

can show that $\eta_{2,1}$ also diverges like $1/a^2$, using arguments similar to those discussed in Sect. 3.1. The $\eta_{2,1}$ dependent terms are thus new examples of Corollary 2.

The subtraction of power divergences based on Eq. (2.4) still goes through unchanged. Explicitly, we find that

$$\mathcal{F} = \mathcal{F}\Big|_{m_{\text{res}}=0} + \frac{32B_0}{(4\pi f)^2 f^2} (\eta_{2,1} - 8\kappa_{6,1}\alpha_2^8) N_s m_{\text{res}}^s, \quad (3.20)$$

$$\langle \pi^+ | \mathcal{Q}_{\text{sub}} | K^+ \rangle = \langle \pi^+ | \mathcal{Q}_{\text{sub}} | K^+ \rangle \Big|_{m_{\text{res}}=0} - \frac{32B_0^2 m^v}{(4\pi f)^2 f^2} \eta_{14} N_s m_{\text{res}}^s. \quad (3.21)$$

This result shows that η_{14} is finite. We also expect that $\eta_{2,1}^{\text{sub}} = \eta_{2,1} - 8\kappa_{6,1}\alpha_2^8$ is a new finite combination of LECs, conform Conjectures 1 and 2.

Of course there are corrections to these results: Eq. (3.12), which expresses the physical pseudo-scalar mass in terms of chiral-lagrangian parameters at NLO, gets modified by the κ LECs defined in Eq. (3.17). Also the chiral logarithms get modified: they are those of ref. [12], with the proviso that now $M_{SS}^2 = 2B_0(m^s + m_{\text{res}}^s)$. The corresponding \mathcal{O}_2 matrix elements needed for the subtraction get new contributions from the m_{res}^s dependence of the strong chiral lagrangian to NLO. However, none of these corrections changes the conclusion that the subtraction procedure still works. The underlying reason is that the operator \mathcal{O}_2 in Eq. (2.2) is still uniquely the only lower-dimension operator that \mathcal{Q} can mix with.

The situation changes if we now also let m_{res}^v be non-zero. In that case, also the valence chiral symmetry in Eq. (2.1) gets broken, and another bilinear operator $\mathcal{O}'_2 = 2m_{\text{res}}^v \bar{s}d$ appears which can mix with \mathcal{Q} and \mathcal{O}_2 . Let us see how this works in ChPT, again omitting mass and wave-function renormalizations, as well as chiral logarithms. Instead of Eqs. (3.18) and (3.19) we find

$$\begin{aligned} \langle 0 | \mathcal{Q} | K^0 \rangle &= \langle 0 | \mathcal{Q} | K^0 \rangle \Big|_{m_{\text{res}}=0} \\ &+ \frac{16iB_0^2(m_s - m_d)}{(4\pi f)^2 f} (\eta_{2,1} N_s m_{\text{res}}^s + 2\eta_{1,1} m_{\text{res}}^v), \end{aligned} \quad (3.22)$$

$$\begin{aligned} \langle \pi^+ | \mathcal{Q} | K^+ \rangle &= \langle \pi^+ | \mathcal{Q} | K^+ \rangle \Big|_{m_{\text{res}}=0} + \frac{8B_0 m_{\text{res}}^v}{f^2} (\alpha_1^8 - \theta_2) \\ &- \frac{32B_0^2 m_{\text{res}}^v}{(4\pi f)^2 f^2} \left((2\beta_{10}^8 + \beta_{11}^8) m^v + \beta_{14}^8 \sum_i m_i^s \right) \\ &- \frac{32B_0^2 (m^v + m_{\text{res}}^v)}{(4\pi f)^2 f^2} \left(\eta_{14} N_s m_{\text{res}}^s + (2\eta_{10} + \eta_{11}) m_{\text{res}}^v \right) \\ &- \frac{32B_0^2 m^v}{(4\pi f)^2 f^2} \left(\eta_{2,1} N_s m_{\text{res}}^s + 4(\eta_{1,1} + \eta_{3,1}) m_{\text{res}}^v \right) \\ &- \frac{32B_0^2 m_{\text{res}}^v}{(4\pi f)^2 f^2} \left(\eta_{2,3} N_s m_{\text{res}}^s + 2(\eta_{1,2} + \eta_{3,2}) m_{\text{res}}^v + \eta_{2,2} \sum_i m_i^s \right). \end{aligned} \quad (3.23)$$

The terms involving α_1^8 or β_i^8 arise because the physical (tree-level) valence-meson mass gets modified to $M_{phys}^2 = 2B_0(m^v + m_{\text{res}}^v)$.

The problem one faces when $m_{\text{res}}^v \neq 0$ comes from the fact that two power-divergent subtractions (both of order $1/a^2$) are needed now, because of the presence of the two lower-dimension operators \mathcal{O}_2 and \mathcal{O}'_2 . An analysis following the lines of Sect. 3.1 shows that the LECs θ_2 , $\eta_{1,i}$, $\eta_{2,i}$, $\eta_{3,i}$ and η_{10} all are expected to diverge as $1/a^2$. Performing only one subtraction with \mathcal{O}_2 would still leave $1/a^2$ divergences in the once-subtracted matrix elements. The only way out is to define a twice-subtracted operator

$$\mathcal{Q}_{\text{two-sub}} = \mathcal{Q} - \mathcal{F}\mathcal{O}_2 - \mathcal{F}'\mathcal{O}'_2, \quad (3.24)$$

for which *all* matrix elements are finite, using two independent subtraction conditions.

The terms that depend only on m_{res}^v or m_{res}^s in the $K^+ \rightarrow \pi^+$ amplitude are in principle not a problem, since they can be separated out by varying m^v and m_i^s , and thus be discarded. But, due to the divergent LECs β_{10}^8 , $\eta_{1,1}$, $\eta_{3,1}$ and η_{10} , the slope of $\langle \pi^+ | \mathcal{Q} | K^+ \rangle$ as a function of m^v , even after subtracting $\langle \pi^+ | \mathcal{O}_2 | K^+ \rangle$ with \mathcal{F} determined from Eq. (2.4), remains power divergent. This magnifies the effect of m_{res}^v , which therefore will need to be small enough to keep this systematic error under control. Of course, the m_{res}^s dependence also introduces an error in the determination of α_1^8 , but this error does not get magnified by $1/a^2$ if $m_{\text{res}}^v = 0$ (*cf.* Eq. (3.21)). The conclusion is that the demand for good chiral symmetry in the valence sector is much more stringent than in the sea sector.

As mentioned, the results of Eqs. (3.22) and (3.23) are not complete without chiral logarithms and mass and wave-function renormalizations. But these “decorations” do not alter our conclusions on the demand on the smallness of m_{res}^v .

4. Bounds

In this section we will address the question: In order that the systematic error due to neglecting m_{res} effects will be at the 1% level, how small should m_{res}^v and m_{res}^s be? Obtaining such bounds requires us to assume something on the magnitude of m_{res} -dependent contributions, relative to the “typical” size of NLO effects in ChPT. To account for the possible occurrence of numerically large LECs we will include a “safety margin” of a factor 10. Namely, we will require that the magnitude of the neglected terms is 1‰ (0.1%) when LECs assume their “typical” anticipated magnitude. We will apply similar considerations to other systematic effects such as (logarithmic) operator mixings and scaling violations.

4.1 How small should m_{res}^v be? (Observation 3)

The method of constructing $K \rightarrow \pi\pi$ matrix elements from $K \rightarrow \pi$ and $K \rightarrow 0$ is highly vulnerable to any non-zero m_{res}^v because, as we discussed in Sect. 3.2, for $m_{\text{res}}^v \neq 0$, it takes *two* subtractions to remove all the power divergences. Once-subtracted matrix elements will therefore still contain power-divergent terms.

The magnitude of the un-subtracted $K^+ \rightarrow \pi^+$ matrix element is parametrically of order $(1/a^2)(B_0 m/f^2)$. Here and below, m should be understood as a shorthand for the linear combination of valence-quark masses relevant for the specific matrix

element. In any given numerical computation, the magnitude of the subtracted matrix element can be written as $(\Delta/a^2)(B_0m/f^2)$. Quenched simulations [6, 9] with $a^{-1} \sim 2$ GeV find that Δ is a few percent,¹⁴ and we will use $\Delta \approx 1\%$ in our bounds.

Before we derive our bound, let us comment on the situation if one considers only LO in ChPT. The LEC α_1^8 is extracted from the slope of the once-subtracted $K^+ \rightarrow \pi^+$ matrix element with respect to m^v , while the divergence associated with \mathcal{O}'_2 (the θ_2 term in Eq. (3.23)) is given by the intercept. Since the slope is independent of the intercept, this procedure effectively amounts to doing both subtractions at the same time at LO. See *e.g.* Fig. 25 of ref. [6].¹⁵ As we showed in Sect. 3.2, this is an artifact of LO ChPT, and not a valid procedure at NLO. The fact that terms at NLO compete with LO terms does not indicate a failure of ChPT. What we have here is a situation where a *divergent* NLO contribution competes with a *finite* LO one. The problem would go away had we made two subtractions! In that case, the bound on m_{res}^v would be closer the bound on m_{res}^s (discussed in Sect 4.2 below). We re-examine this issue in Sect. 5.

At $m_{\text{res}}^v \neq 0$, once-subtracted matrix elements will have NLO power divergences which are parametrically of order $(1/a^2)(B_0m/f^2)B_0m_{\text{res}}^v/(4\pi f)^2$. Our bound follows from the requirement that this will not exceed 1‰ of the physical answer. Dropping common factors, we obtain

$$B_0m_{\text{res}}^v/(4\pi f)^2 \leq 0.001\Delta \approx 10^{-5}. \quad (4.1)$$

It may be more useful to re-express this bound in terms of the quantity am_{res}^v , which is the dimensionless residual mass measured directly in the simulation. Both B_0 and $4\pi f$ are roughly of order 1 GeV, and the same is true for the inverse lattice spacing used in numerical simulations. Hence, in practice, $B_0/(4\pi f)^2 \approx a$ and we may re-write Eq. (4.1) as $am_{\text{res}}^v \leq 10^{-5}$.

Taking $B_0m/(4\pi f)^2$ as the chiral expansion parameter is based on the known values of NLO strong LECs. The LECs λ_i (*cf.* Eq. (3.10)) suitable for this parameterization are indeed $O(1)$. What would happen if it turns out that, say, $B_0m/(4\pi f)^2$ (rather than $B_0m/(4\pi f)^2$) is the “true” chiral expansion parameter for the relevant weak matrix elements? Since $4\pi \approx 10$, would this change our estimate by the same amount? The answer is no! It is precisely because of this uncertainty that we have already included the safety margin of 10 in our estimate. Thus, requiring that am_{res}^v be of order 10^{-6} would amount to a safety margin of a factor 100.

4.2 How small should m_{res}^s be? (Observation 4)

From now on we will assume that $am_{\text{res}}^v \leq 10^{-5}$, and, hence, that we may use all the results derived for $m_{\text{res}}^v = 0$. As for m_{res}^s , we may or may not neglect it the analysis of a simulation, and the resulting error will be slightly different in each case.

Let us first assume that m_{res}^s is neglected, namely, one performs the ChPT matching at $m_{\text{res}}^v = m_{\text{res}}^s = 0$. The obvious advantage of this choice is that the analysis

¹⁴This is consistent with $\Lambda_{QCD}^2 \approx 0.01/a^2$.

¹⁵From this figure one deduces that, like α_2^8 , the LO LEC θ_2 (Eq. (3.16)) is parametrically of order $1/a^2$, as expected.

involves the minimal number of NLO parameters as dictated by continuum ChPT. The neglected m_{res}^s -dependent terms are again NLO, but this time they contain no power divergence, because the single subtraction of Sect. 2 removes the entire power divergence for $m_{\text{res}}^v = 0$. We already know from the LO analysis that the magnitude of a “typical” finite LEC is Δ times the magnitude of a “typical” power-divergent LEC. The neglected terms are therefore of order $(\Delta/a^2)(B_0 m/f^2)B_0 m_{\text{res}}^s/(4\pi f)^2$, and this should be less than 1‰ times the LO finite result. Dropping all common factors (including Δ this time) gives rise to the simple result

$$B_0 m_{\text{res}}^s/(4\pi f)^2 \leq 0.001, \quad (4.2)$$

As before, this bound is the same as $am_{\text{res}}^s \leq 0.001$ if $a^{-1} \sim 1$ GeV.

Compared to Eq. (4.1), the bound (4.2) is far less stringent. We now consider also short-distance systematic errors induced by neglecting m_{res}^s . This includes mixings between dimension-six operators that are allowed by the symmetry of Eq. (2.1) but not by the full PQ symmetry (3.1). Operator mixings are determined (*e.g.* using the RI NPR method [6]) at off-shell momenta of roughly $p \approx 1/a$. The resulting “wrong-chirality” operator mixing will therefore be at most of order am_{res}^s , and requiring this to be a 1‰ effect (safety margin included) we again end up with $am_{\text{res}}^s \leq 0.001$.¹⁶

We next consider what scaling violations are induced at non-zero m_{res}^s . At $m_{\text{res}}^v = 0$, domain-wall fermions have only $O(a^2)$ scaling violations. Since $a\Lambda_{QCD} \approx 0.1$, this is a 1‰ effect. For $m_{\text{res}}^s \neq 0$ we may have $O(a)$ scaling violations coming from the dimension-five operator $\bar{q}\sigma_{\mu\nu}F_{\mu\nu}q$. Exact chiral symmetry forbids this operator, hence it can at most arise with a coefficient of order am_{res}^s . Requiring that this effect will be smaller than $0.1(a\Lambda_{QCD})^2$ we end up with the same bound as before.

In summary, taking known sources of systematic error into account we conclude that, provided $am_{\text{res}}^s \leq 0.001$, all m_{res}^s effects can be completely neglected and the resulting error due to m_{res}^s should be at the 1‰ level.

Of course, several independent 1‰ errors might accumulate to a somewhat bigger error. If one does ChPT at non-zero m_{res}^s , the systematic error generated by the ChPT matching will be entirely due to NNLO effects. However, this would require more measurements to extract the new linear combinations of NLO LECs that occur in $K^0 \rightarrow \pi^+\pi^-$ when $m_{\text{res}}^s \neq 0$.

We anticipate that the numerical calculation of dimension-six operator mixing should be feasible assuming only the symmetry of Eq. (2.1) which takes into account that $m_{\text{res}}^s \neq 0$. (See *e.g.* the NPR mixing matrix in Tables 12,13 of ref. [6], where mixings that violate $SU(3)_L \times SU(3)_R$ are not neglected.)

Quark masses commonly used in numerical simulations are typically in the range of few times 10 MeV, and so $am_{\text{res}}^s \approx 0.001$ may already account for up to 10% of the physical sea-quark mass. We thus believe that, no matter what, one should avoid residual masses (be it m_{res}^s or, certainly, m_{res}^v) larger than 0.001.

The good chiral symmetry of domain-wall fermions enhances a quenched pathology: due to the absence of the fermion determinant, contributions of physical zero modes grow like the inverse quark mass. While methods have been devised to deal

¹⁶This bound is obtained directly in terms of am_{res}^s without using the “translation” $B_0/(4\pi f)^2 \approx a$.

with this problem in the quenched theory [18], clearly the only true solution is to un-quench. The pathology is removed when the physical sea and valence masses are set to the same value. To LO, this means

$$m_i^{\text{ph}} = m_i^v + m_{\text{res}}^v = m_i^s + m_{\text{res}}^s. \quad (4.3)$$

Observe that this does *not* require that m_{res}^v and m_{res}^s be equal. When m_{res}^v is negligibly small, this amounts to tuning the valence-quark mass m_i^v to $m_i^s + m_{\text{res}}^s$. In a numerical simulation, the correct procedure is to tune the valence-pion mass to the sea-pion mass. Another advantage of this choice is that enhancement of finite-volume effects is avoided [14].

5. Discussion

Our analysis shows that, because power divergences are encountered in the valence sector only, the chiral-symmetry requirements on valence quarks are much more stringent in comparison to sea quarks. To keep systematic errors due to chiral symmetry violation at the 1% level, we estimate that one needs $am_{\text{res}}^v \leq 10^{-5}$ and $am_{\text{res}}^s \leq 10^{-3}$ at $a^{-1} \sim 2$ GeV. The obvious conclusion is to adopt the strategy of using different DWF actions for the two sectors. A more economic DWF action can, and should, be chosen for the sea sector; it is the sea sector that costs most of the computational effort, and at the same time this is where a much larger residual mass can be tolerated!

The simplest way to choose different DWF actions for the two sectors is to take $L_5^s < L_5^v$. This choice is a hybrid scheme in the sense of ref. [4], with symmetry group $G_{\text{sea}} \times G_{\text{valence}} = U(N_s) \times U(N_v|N_v)$. For $L_5^s = L_5^v$ the symmetry group enlarges to the group $U(N_v + N_s|N_v)$ [10], and in that case the theory is what is usually referred to as partially quenched, rather than hybrid. While these are all rather trivial statements, they have one relevant consequence: The most general theory, with free parameters $m_q^{v,s}$ and $L_5^{v,s}$, rigorously contains fully unquenched QCD as a special case, by choosing $m_q^v = m_q^s$, $L_5^v = L_5^s$. However, while simulations can easily obtain data points for $m_q^v = m_q^s$, this is less likely the case for the size of the fifth dimension. The problem is that, as we have seen, choosing $L_5^v = L_5^s$ for affordable values of L_5^s is unlikely to yield the high chiral accuracy needed in the valence sector. Note that one might choose hybrid schemes in which the valence- and the sea-quark DWF operators differ not only in the values of L_5 or m_q , but also in other ways (see below).

Of course, spectral functions extracted from the mixed theory, in which quark masses have been tuned such that Eq. (4.3) holds, may suffer from violations of positivity at non-zero lattice spacing. However, provided the bounds discussed in Sect. 4 are satisfied, implying that $a(m_{\text{res}}^s - m_{\text{res}}^v)$ errors are not bigger than a^2 errors, this will show up as just another source of $O(a^2)$ scaling violations. If Eq. (4.3) does not hold, one expects unitarity violations to occur also in the continuum limit as in any partially-quenched theory.

In the quenched case, changing the gauge action (to Iwasaki [19] or to DBW2 [20]) turned out to be enough to push m_{res} to negligibly small values. In the dynamical

DWF case [21], fiddling only with the gauge action gives rise to $m_{\text{res}} = m_{\text{res}}^s$ values which at present are marginally within our bound for two flavors, and larger than our bound for three flavors. Moreover, trying to use exactly the same DWF action for the valence sector would entail violating our m_{res}^v bound by several orders of magnitude.

The inherent reason for the larger m_{res} values obtained in the dynamical case is the screening effect of the sea quarks, requiring a larger bare coupling in order to maintain the same lattice cutoff. This larger bare coupling pushes one closer to the Aoki phase [22, 23, 24]. Inside the Aoki phase, DWF and overlap fermions [25] cannot be used because it is impossible to maintain both chirality and locality [26, 17].

To meet the bounds derived in this paper it is necessary to use better DWF actions (for both fermions and Pauli-Villars fields). We recall that the basic elements that go into a DWF construction are the four-dimensional “kernel” (for standard DWF, a super-critical Wilson operator) and the way the fermions are allowed to hop in the fifth dimension (for standard DWF, a free one-dimensional Wilson operator). Both play a role in the resulting Ginsparg-Wilson (GW) operator [27] obtained in the chiral limit $L_5 \rightarrow \infty$, and faster approach to the DWF chiral limit often gives rise to a GW operator with better locality properties. While the study of improved DWF actions is outside the scope of this paper, we briefly list several existing proposals.

1. Accelerated convergence to the chiral limit [28]. This method changes the couplings in the fifth dimension, in effect applying a Möbius transformation to the Wilson kernel. It includes as special cases the standard DWF formulation [2] and the “truncated overlap” of ref. [29]. It shows promising results. It can be applied to both the sea- and the valence-quark sectors. The difference between the sea and the valence DWF actions can come not only from (m and) L_5 but also from two optimization parameters, see ref. [28] for details.

2. Modified four-dimensional kernel. Modifications have been proposed based on the rate of approach to the chiral limit in perturbation theory [30], and on approximate solutions [31] of the GW relation which also improve the locality of the resulting overlap operator. These methods are again applicable to both sea and valence quarks.

3. Modified Pauli-Villars action [32]. This method is relevant only to the sea-quark sector. It aims to suppress the Boltzmann weight of dislocations that give rise to low-lying eigenmodes of the Wilson kernel. These eigenmodes allows for un-suppressed propagation in the fifth dimension, and are the dominant non-perturbative source of chiral symmetry violation.

4. “Projection method” [33]. In this method, one adds to the DWF Dirac operator terms proportional to the projectors on low-lying eigenmodes of the Wilson kernel. This in effect raises the corresponding eigenvalues and eliminates the associated un-suppressed propagation in the fifth dimension. The method is consistent so long as these eigenmodes are exponentially localized. The method could be prohibitively expensive for the sea sector. As for the valence sector, the extra cost of computing the projection terms should be small compared to the cost of generating the dynamical configuration itself. Under favorable conditions, “projecting out” a relatively small number of Wilson eigenmodes can lead to a significant reduction of m_{res}^v .

5. Another method which would be prohibitively expensive for the sea sector, but can be used in the valence sector, is to smear the gauge links before plugging them into the DWF Dirac operator [34]. Again, this removes many of the dislocations that would otherwise give rise to low-lying eigenmodes of the Wilson kernel.

Once dynamical DWF configurations with $am_{\text{res}}^s \leq 10^{-3}$ have been produced there is a good chance that, with all the extra “tricks” available in the valence sector, it will be possible to meet the valence-sector bound $am_{\text{res}}^v \leq 10^{-5}$ as well, at affordable cost.

In Sect. 3 we concluded that, when $m_{\text{res}}^v = 0$, the divergent part of \mathcal{F} is $\mathcal{F}_2/a^2 = 8\alpha_2^8/f^2$. Similarly, if we consider the twice-subtracted operator (Eq. (3.24)) needed when $m_{\text{res}}^v \neq 0$, we have that $\mathcal{F}_2/a^2 = 8\alpha_2^8/f^2$ as before, while $\mathcal{F}'_2/a^2 = 8\theta_2/f^2$. This follows from the LO analysis, but should remain true to NLO if indeed the NLO corrections to \mathcal{F} and \mathcal{F}' are always finite (*cf.* Conjecture 2). This suggests that a twice-subtracted operator may be defined by first performing one subtraction by imposing Eq. (2.4), and then performing the second subtraction, $\mathcal{Q}_{\text{two-sub}} = \mathcal{Q}_{\text{sub}} - \mathcal{F}'\mathcal{O}'_2$, by imposing $\langle \pi^+ | \mathcal{Q}_{\text{two-sub}} | K^+ \rangle = 0$ in the limit that the explicit valence quark mass is zero. The ChPT matching should then involve the corresponding NLO result $\mathcal{F}' = 8\theta_2/f^2 + O(m_{\text{res}}, m^s)$, where the NLO terms are again finite. Observe that, unlike the first subtraction, the second subtraction cannot be done without relying on ChPT to some order. This brings in new uncertainties (for instance, the convergence of the chiral extrapolation). Given these uncertainties, we believe that the necessary bound on am_{res}^v will fall somewhere in between 10^{-5} and 10^{-3} in that case.

Finally, it is interesting to see whether the considerations on the interplay of power divergences and chiral symmetry presented in this paper carry over to other fermion methods. For instance, as an alternative to using DWF, efforts are under way to use staggered valence quarks to determine $K \rightarrow \pi\pi$ from $K \rightarrow \pi$ matrix elements [35]. Naively, one expects that bounds on the maximum tolerable Goldstone-boson mass splittings coming from taste symmetry breaking would have to be similarly stringent as those on m_{res}^v . The reason is that taste symmetry breaking in the valence sector might again lead to the need to perform more than one power-like subtraction. However, in this case the problem is avoided by using only the exact Goldstone bosons on the external lines of the matrix elements under consideration.

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Appendix A. Systematics of chiral symmetry violations

In this paper, we assumed that finite- L_5 chiral symmetry violations can be treated in ChPT by introducing a spurion field associated with the “residual mass.” While the bare quark mass is a small parameter explicitly present in the DWF action, the same is not true for the residual mass; its smallness is a dynamical result. In this Appendix we discuss this dynamics in some detail, finding that a systematic treatment of residual chiral symmetry violations requires several spurions. However, this will not modify the NLO analysis of Sect. 3 (except for an inessential modification to Eq. (3.23)) and, thus, it has no effect on our conclusions.

At finite L_5 , the DWF’s PCAC relation takes the form [2]

$$\partial_\mu^- J_{5\mu}^a = 2mJ_5^a + 2J_{5q}^a, \quad (\text{A.1})$$

where for simplicity we assume equal quark masses. Here $J_{5\mu}^a$ is a DWF’s partially-conserved non-singlet axial current and ∂_μ^- is the backward lattice derivative. J_5^a is built out of fermion field residing on the boundaries, and interpolates a (continuum) pseudo-scalar density. J_{5q}^a is a lattice artifact that involves fermion fields residing inside the five-dimensional “bulk,” half-way between the boundaries. The notion of a residual mass comes from the fact that the leading long-distance effect of J_{5q}^a can be expressed as $J_{5q}^a \approx m_{\text{res}} J_5^a$. This motivated the definition of the spurion M_{res} in Eq. (3.14). In this appendix we address the legitimacy of this approximation.

Propagation in the fifth dimension is governed by a transfer matrix T , from which a hamiltonian $\tilde{H} = -\log(T)/a_5$ may be defined, where a_5 is the spacing in the fifth dimension. \tilde{H} is closely related to the Wilson operator, and in particular the two operators share identical zero modes. Each eigenmode of \tilde{H} can be characterized as extended or localized. Outside the Aoki phase, one expects the localized eigenmodes to lie below a mobility edge $\tilde{\lambda}_c > 0$, above which the eigenmodes are extended. Following ref. [17] we will now separately discuss the chiral symmetry violations arising from the extended and from the localized modes, in that order.

In the presence of extended modes only, low-energy quark modes will have a factorized wave function $\psi_{DWF}(x, s) \rightarrow q_R(x)\chi(s) + q_L(x)\chi(L_5 + 1 - s)$ where $s = 1, 2, \dots, L_5$ is the fifth coordinate and $q_{R,L}(x) = \frac{1}{2}(1 \pm \gamma_5)q(x)$ is an effective four-dimensional quark field. This was derived in perturbation theory [30], and is expected to hold non-perturbatively as well. The fifth-coordinate wave function $\chi(s)$ is dominated by the extended modes near the mobility edge,¹⁷ and is given by $\chi(s) \sim \exp(-a_5 s \tilde{\lambda}_c)$. Since the left-handed and right-handed quarks reside on opposite boundaries, each chirality flip will involve a factor of $\chi(L_5) \sim \exp(-a_5 L_5 \tilde{\lambda}_c)$ when $m = 0$. This resembles a mass insertion with $\chi(L_5)$ as the mass. Hence we can

¹⁷In perturbation theory the mobility edge is equal to the gap of the free \tilde{H} . See also the last paper of ref. [17].

account for it by introducing a mass-spurion M_{ext} with expectation value

$$M_{\text{ext}} = \text{diag}(m_{\text{ext}}^v, \dots, m_{\text{ext}}^s, \dots, m_{\text{ext}}^v, \dots), \quad (\text{A.2})$$

where

$$am_{\text{ext}}^v \sim \exp(-a_5 L_5^v \tilde{\lambda}_c^v), \quad (\text{A.3})$$

and similarly for m_{ext}^s .

We next turn to the localized modes. Among these, the most dangerous are the zero modes of \tilde{H} , which give rise to un-suppressed propagation between the two boundaries. At a given L_5 , the term “zero modes” stands here for all modes with eigenvalue $|\lambda| \lesssim 1/L_5$. The probability (per unit volume) to encounter a zero mode is roughly given by $\tilde{\rho}(0)/L_5$, where $\tilde{\rho}(\lambda)$ is the spectral density of \tilde{H} , and $1/L_5$ accounts for the energy interval.¹⁸ Evidently, the smallness of this effect hinges on having a small $\tilde{\rho}(0)$. As before, we introduce a new mass-spurion M_{lcl} with

$$M_{\text{lcl}} = \text{diag}(m_{\text{lcl}}^v, \dots, m_{\text{lcl}}^s, \dots, m_{\text{lcl}}^v, \dots), \quad (\text{A.4})$$

in which

$$am_{\text{lcl}}^v \sim a^4 \tilde{\rho}^v(0)/L_5^v, \quad (\text{A.5})$$

etc. However, for the chiral symmetry violations coming from localized modes, this is not the whole story. Once a zero mode is found some place in the configuration, it allows for quarks of any flavor to propagate from one boundary to the other with no “penalty.” Since the process is confined to the space-time region occupied by the zero mode, we anticipate that it can be described in terms of a local effective multi-fermion interaction. Given *e.g.* N_s sea quarks, a single zero mode can certainly give rise to effective vertices containing $2, 4, \dots$, up to $2N_s$ fermions, which induce one chirality flip per flavor.¹⁹

The Symanzik action is a continuum effective action in which the lattice artifacts occur in an expansion in the lattice spacing. In this effective action the multi-fermion vertices discussed above will have dimensionful coupling constants, each of which will be roughly equal to the common factor $\tilde{\rho}(0)/L_5$, times an appropriate power of the lattice spacing. To account for this effect in ChPT [23, 4], we thus need to introduce a third spurion W transforming again in the same way as a mass spurion, and having an expectation value

$$W = \text{diag}(w, \dots, w, \dots, w, \dots), \quad (\text{A.6})$$

with

$$w \sim a^3. \quad (\text{A.7})$$

Thus, *e.g.* a sea-sector $2n$ -fermion vertex (which induces n chirality flips) will occur at order $m_{\text{lcl}}^s a^{3(n-1)}$ in the chiral expansion.

We end up with the following two rules for residual chiral symmetry violations in ChPT:

¹⁸This corresponds to the third scenario described in appendix C.2 of ref. [30].

¹⁹This might be thought of as reminiscent of the 't Hooft vertices induced by instanton zero modes. We leave open how many chirality flips can be induced by a single zero mode of \tilde{H} in the case at hand.

1. The effects are accounted for by the three mass spurions M_{ext} , M_{lcl} and W .
2. The spurion W cannot occur except in terms that already contain at least one power of M_{lcl} . (More precisely, this is true separately for the valence and sea sectors.)

The values of all three spurions are to be defined in the limit in which the explicit quark mass has been set equal to zero.²⁰ ChPT will then automatically take care of the dependence of the residual mass on the explicit quark masses. Numerically, for the range of quark masses used in simulations, the variation in the residual mass is found to be at the level of a few percent [19, 20], showing that it is indeed consistent to treat it as a higher order effect in ChPT.

For small L_5 the dominant chiral symmetry violating effects will come from extended modes. Since this effect is damped exponentially, above some value of L_5 the localized zero modes will take over as the dominant source of chiral symmetry violations. Their effects have a lot in common with the chiral symmetry violations of Wilson fermions. The crucial difference is that, for DWF, these effects have a low probability given by $\tilde{\rho}(0)/L_5$. This is the origin of Rule 2.

It has been suggested that the treatment of DWF chiral symmetry violations in ChPT can be based on promoting the fifth-direction links located exactly in the middle of the fifth dimension to a spurion Ω [16]. However, adopting the more elaborate scheme of spurions developed above allows one to account more faithfully for the magnitude of residual chiral symmetry violations coming from the different dynamical sources.

Were it not for W , we could define $M_{\text{res}} = M_{\text{ext}} + M_{\text{lcl}}$ and the ChPT treatment would be reduced to the single M_{res} spurion introduced in Eq. (3.14). While in general this is not the case, thanks to Rule 2 it remains true that the leading residual-mass dependence must be through the sum $M_{\text{ext}} + M_{\text{lcl}}$. Let us now re-examine the results of Sect. 3. First, for $m_{\text{res}}^v = 0$ (*i.e.* for $m_{\text{ext}}^v = m_{\text{lcl}}^v = 0$), the results depend linearly on m_{res}^s . The distinction between the contributions of extended and localized modes therefore plays no role to NLO when $m_{\text{res}}^v = 0$. To follow the above rules, we would only need to perform the trivial substitution $m_{\text{res}}^s = m_{\text{ext}}^s + m_{\text{lcl}}^s$.

When m_{lcl}^v is non-zero things get (yet) more complicated compared to Eq. (3.23). This equation is quadratic in m_{res}^v . Therefore, apart from setting $m_{\text{res}}^v = m_{\text{ext}}^v + m_{\text{lcl}}^v$, there are additional NLO terms proportional to $m_{\text{lcl}}^v a^3$. This, however, has no effect on the bound (4.1), which originates from the terms in Eq. (3.23) proportional to $m_{\text{res}}^v m^v$.

So far, we have encountered no difference between the way the explicit-mass spurion M and the new spurion M_{ext} enter ChPT. This raises the question whether one can trade M and M_{ext} for a single spurion $M' = M + M_{\text{ext}}$. The answer depends on the context. For pure-QCD observables (such as spectrum), the only distinction is that the LECs corresponding to M and to M_{ext} will in general exhibit different scaling violations. This is best seen by considering the effective four-dimensional lattice Dirac

²⁰One should be able to extract m_{ext} and m_{lcl} from a fit of m_{res} as a function of L_5 .

operator obtained by integrating out the five-dimensional bulk modes [36].²¹ This Dirac operator will involve a new mass term with coefficient $m_{\text{ext}} \sim \exp(-a_5 L_5 \tilde{\lambda}_c)$. However, in addition it will contain irrelevant terms transforming in the same way as a mass term, with coupling constants of order $\exp(-a_5 L_5 \tilde{\lambda}_c)$. Since there are no corresponding irrelevant interactions for the explicit mass term, the resulting scaling violations will be different.

However, when insertions of the effective weak hamiltonian are considered, one encounters the power divergences which are the main topic of this paper. In this case, the numerical results [6, 9] show that the difference between the LECs corresponding to m^v and to m_{res}^v , such as for example α_2^8 and θ_2 , is roughly of the same size as these LECs. Therefore it is not possible to combine the explicit-mass spurion M with any of the residual-mass spurions.

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²¹Note that localized modes can, in principle, be avoided by imposing an admissibility condition [26].

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