Unphysical Operators in Partially Quenched QCD

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We point out that the chiral Lagrangian describing pseudo-Goldstone bosons in partially quenched QCD has one more four-derivative operator than that for unquenched QCD with three flavors. The new operator can be chosen to vanish in the unquenched sector of the partially quenched theory. Its contributions begin at next-to-leading order in the chiral expansion. At this order it contributes only to unphysical scattering processes, and we work out some examples. Its contributions to pseudo-Goldstone properties begin at next-to-next-to-leading order, and we determine their form. We also determine all the zero and two derivative operators in the $O(p^6)$ partially quenched chiral Lagrangian, finding three more than in unquenched QCD, and use these to give the general form of the analytic next-to-next-to-leading order contributions to the pseudo-Goldstone mass and decay constant. We discuss the general implications of such additional operators for the utility of partially quenched simulations.

I. INTRODUCTION

Chiral perturbation theory ($\chi$PT) allows analytic calculations of low-energy QCD processes, results of which are given in terms of a number of undetermined constants, e.g. the Gasser-Leutwyler coefficients. These low-energy constants are fundamental QCD parameters that govern physical properties such as masses and scattering amplitudes. Lattice QCD provides a method for determining them from first principles, as long as simulations are done at small enough quark masses that $\chi$PT (typically at next-to-leading order) is a good approximation. In practice, however, simulating light dynamical quarks is computationally expensive, and there is a limited range of quark masses where both lattice simulations are feasible and $\chi$PT is applicable.

This situation can be improved using the partially quenched (PQ) approximation, in which valence quarks (those which appear in external states) and sea quarks (those which appear in loops) are allowed to have different masses. To ensure that valence quarks exist only in external states, valence quarks have bosonic ghost quark partners of equal mass. The presence of ghosts means that the PQ theory as a whole is unphysical, although the sea quark

![FIG. 1: Parameter space of partially quenched theories. Physical theories, such as QCD, live on the diagonal line. Lattice simulations have been done with “light” quark masses as low as $\sim m_{\text{strange}}/8$. Note that this plot is schematic, since there are actually multiple valence and sea quarks, all of which can have different masses.](arXiv:hep-lat/0310012v2_7Jan2004)

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sector contained within it is physical. Consideration of PQ theories expands the parameter space available for lattice simulations and comparison to χPT, as shown in Fig. II.

In Refs. 1, 2 it is argued that PQ QCD can be used for a quantitative determination of the QCD low-energy constants. The primary assumption is that a generalization of χPT can be used to describe the low-energy behavior of PQ QCD. This theory, called PQχPT, must contain all of the operators of unquenched χPT in order to describe the behavior of the unquenched sector. Quark mass dependence in both χPT and PQχPT is explicit, so the coefficients in the Lagrangian depend only on the number of quarks. Therefore the coefficients of operators in the unquenched chiral Lagrangian are identical to those of corresponding operators in the PQ chiral Lagrangian for $N_{\text{sea}} = 3$.1

To make use of this observation one fits results from PQ simulations to the predictions of PQχPT and thereby determines the low-energy constants. Particular quantities studied in Refs. 1, 2 were next-to-leading order (NLO) PGB masses and decay constants, as well as the hairpin vertex. It was asserted for these calculations that there are no new operators through NLO in the PQ chiral Lagrangian, so that no additional low-energy constants are needed at this order. Here we show that Refs. 1, 2 missed one operator in the NLO Lagrangian, and explore the consequences. The existence of additional operators does not fundamentally change the approach, it does necessitate an elaboration of the program of using PQ QCD to determine low energy constants.

The general situation is as follows. The PQ chiral Lagrangian contains two types of operators: first, those which, in the sea quark sector, reduce to operators present in the QCD chiral Lagrangian, and whose coefficients are thus identical to those in QCD, and, second, operators which vanish in the sea quark sector. We call the latter unphysical operators. Their coefficients are additional unphysical constants needed to describe the low-energy behavior of the PQ theory. These appear first at NLO in chiral perturbation theory, with increasing numbers required as one works at higher order. In general, both types of operator need to be taken into account when matching forms calculated in PQχPT to PQ lattice data. It turns out, however, that for masses, decay constants and the hairpin vertex, the new operators do not contribute until next-to-next-to-leading order (NNLO). Thus the results of Refs. 1, 2 are unchanged.

This paper constitutes a preliminary investigation of the impact of the unphysical operators on the utility of PQ QCD. It is organized as follows. In Sec. II, we derive the existence and form of the new, linearly-independent four-derivative operator present in the PQ chiral Lagrangian at NLO. We explore the consequences of this operator in Sec. III by discussing the type of meson scattering processes to which it contributes. In Sec. IV we continue the study of Refs. 1, 2 by calculating the leading contribution of this operator to meson masses and decay constants, which appear first at NNLO. This raises the general issue of extending the approach of using PQχPT to NNLO. In Sec. V we take another step in this direction by discussing the analytic NNLO corrections to meson masses and decay constants. We determine the operators that contribute, construct a minimal, linearly-independent set, and show which of them vanish in the unquenched sector. Finally, in Sec. VI we summarize our findings, and discuss their general implications concerning the utility of PQ simulations.

II. NEW FOUR-DERIVATIVE OPERATOR IN PQχPT

We first recall the chiral effective Lagrangian describing the properties of the light pseudo-Goldstone boson (PGB) octet in QCD. Spontaneous breakdown of the approximate $SU(3)$ chiral symmetry of QCD by the vacuum,

$$SU(3)_L \times SU(3)_R \to SU(3)_V,$$

leads to an octet of PGBs. They are conveniently collected into an $SU(3)$ matrix,

$$\Sigma = e^{(2i\Phi/f)}$$

$$\Phi = (\Phi_{ij}), \quad i, j = u, d, s$$

$$\text{Tr} (\Phi) = 0,$$

where $f$ is the leading-order meson decay constant. Under chiral symmetry transformations $\Sigma$ transforms as:

$$\Sigma \to L \Sigma R^\dagger$$

1 It is important for this argument that the $\eta'$ can be integrated out of the PQ theory, which is shown in Ref. 2.
\[ L \in SU(3)_L, \quad R \in SU(3)_R \]  
In the meson sector, \( \chi \)PT is an expansion in powers of \( \epsilon^2 \sim m_P^2/(4\pi f)^2 \sim p_P^2/(4\pi f)^2 \). The lowest-order Lagrangian is of \( O(\epsilon^2) \):

\[ \mathcal{L}_2 = \frac{f^2}{4} \text{Tr}(\partial_\mu \Sigma \partial_\mu \Sigma) - \frac{f^2}{4} \text{Tr}(\chi \Sigma^\dagger + \Sigma \chi) \]

Here \( \chi \) is proportional to the quark mass matrix,

\[ \chi_{ij} = \delta_{ij}\chi, \]

and is defined such that the mass of a PGB containing quarks \( i \) and \( j \) is

\[ m_{ij}^2 = \frac{\chi_i + \chi_j}{2} \]

at lowest order. Similarly, the \( O(\epsilon^4) \), or Gasser-Leutwyler, Lagrangian is

\[ \mathcal{L}_4 = -L_1[\text{Tr}(\partial_\mu \Sigma \partial_\mu \Sigma^\dagger)]^2 - L_2[\text{Tr}(\partial_\mu \Sigma \partial_\nu \Sigma^\dagger)\text{Tr}(\partial_\nu \Sigma \partial_\mu \Sigma^\dagger)] - L_3[\text{Tr}(\partial_\mu \Sigma \partial_\nu \Sigma^\dagger \partial_\nu \Sigma \partial_\mu \Sigma^\dagger) + \text{contact terms} \]

It is important to recall that \( SU(3) \) group relations and \( O(\epsilon^2) \) equations of motion were used to reduce the operators in \( \mathcal{L}_4 \) to a minimal, linearly-independent basis.

Partial quenching introduces unphysical, bosonic ghost quarks partners of equal mass for the valence quarks \( A, B, \ldots \):

\[ \Sigma = e^{(2i\Phi/f)} \]

\[ \Phi = (\Phi_{ij}), \quad i, j = A, B, \ldots, 1, 2, \ldots, \overbrace{N_{\text{valence}}}, \overbrace{N_{\text{sea}}}, \overbrace{N_{\text{valence}}} \]

\[ \text{Str}(\Phi) = 0 \]

“Str” indicates supertrace, the graded analog of the trace. The transformation properties of \( \Sigma \) are the same as in Eq. (5), except that the chiral symmetry group becomes a graded group with both commutation and anti-commutation relations:

\[ SU(N_{\text{sea}}) \rightarrow SU(N_{\text{valence}} + N_{\text{sea}}|N_{\text{valence}}). \]

At leading order, the PQ chiral Lagrangian takes the same form as for QCD, Eq. (6), except that traces are replaced with supertraces. There are no additional operators invariant under the new PQ chiral symmetry group. It was asserted in Refs. [1, 2, 3] that the same is true for the NLO Lagrangian, \( \mathcal{L}_4 \). This is in fact incorrect. The number of four-derivative operators in Eq. (10) was reduced from four to three using \( SU(3) \) group relations. This reduction does not occur in the PQ theory, as we now explain.

We can use group theory to determine the number of linearly independent four-derivative operators in \( \mathcal{L}_4 \) in a general \( SU(N|M) \) PQ theory.\(^3\) It is useful to build such terms out the right-handed Lie derivative\(^4\) \( \Sigma^\dagger \partial_\mu \Sigma \). Under the chiral group this transforms as

\[ (\Sigma^\dagger \partial_\mu \Sigma) \rightarrow R (\Sigma^\dagger \partial_\mu \Sigma) R^\dagger, \]

\(^2\) We do not consider the Wess-Zumino-Witten Lagrangian in this paper, since it does not contribute to the processes we study until higher order than we consider.

\(^3\) In standard discussions for \( SU(N) \), the analysis is usually based on the Cayley-Hamilton theorem, from which one can determine relations between products of traces of matrices. This approach does not, however, generalize to graded groups, so we use an alternative method which does generalize.

\(^4\) All terms involving derivatives in \( \mathcal{L}_4 \), Eq. (10), can be written in terms of Lie derivatives by appropriately inserting factors of \( \Sigma^\dagger \Sigma = 1 \).
and thus potentially contains an adjoint and a singlet component. The singlet is absent because the Lie derivative has vanishing supertrace. We can write it as

$$\Sigma^\dagger \partial_\mu \Sigma = i l_\mu (\Phi(x)) \cdot \overline{\tau},$$

where $\tau$ is an $SU(N|M)$ generator, and the vector $l_\mu$ is a real function of $\Phi$ and its derivatives. The four-derivative terms contain four Lie derivatives, with the Lorentz indices necessarily contracted in two pairs, so that the terms have the schematic form

$$(l_\mu \cdot \overline{\tau})(l_\mu \cdot \overline{\tau})(l_\nu \cdot \overline{\tau})(l_\nu \cdot \overline{\tau}).$$

Here group indices are not yet contracted, and the issue is to determine the number of singlets under the chiral group that are contained in this quantity. The product $(l_\mu \cdot \overline{\tau})(l_\mu \cdot \overline{\tau})$ contains all representations arising in the symmetric product of two adjoints. Each of these can be combined to make a singlet with the corresponding representation coming from the other product with $\mu \to \nu$. We conclude that the number of independent singlets that one can make out of right-handed Lie derivatives is given by the number of representations contained in the symmetric product of two adjoints. In fact, this gives all the independent four-derivative terms because all invariants that can be built out of right-handed Lie derivatives can be rewritten in terms of right-handed Lie derivatives alone, using the cyclicity of the supertrace.

Figure 2 shows the symmetric product of two adjoints in $SU(N|M)$. We use the notation for graded Young tableaux of Refs. [5, 6]. There are four representations, all of which are self-conjugate. They can each form a flavor singlet with the same representation in the other pair of adjoints, so there are four linearly-independent operators in the PQ theory. Without the dashed diagonal lines, Fig. 2 is also the symmetric product of two adjoints. Each of these can be combined to make a singlet with the corresponding representation coming from the other product with $\mu \to \nu$. We conclude that the number of independent singlets that one can make out of right-handed Lie derivatives is given by the number of representations contained in the symmetric product of two adjoints. In fact, this gives all the independent four-derivative terms because all invariants that can be built out of four left-handed, or two left-handed and two right-handed, Lie derivatives can be rewritten in terms of right-handed Lie derivatives alone, using the cyclicity of the supertrace.

We conclude that there is one additional four-derivative operator in the PQ chiral Lagrangian, just as there is an additional operator in unquenched theories with four or more flavors.

It is straightforward to determine the form of the new operator. In addition to the three in Eq. (10) with trace replaced by supertrace, we have:

$$\text{Str}(\partial_\mu \Sigma \partial_\nu \Sigma^\dagger \partial^\nu \Sigma \partial^\nu \Sigma^\dagger)$$

For comparison with unquenched QCD, it is convenient to use a linear combination of operators that vanish in the unquenched $SU(3)$ sector of the PQ theory:\cite{5,6}

$$O_{PQ} = \left\{ \text{Str}(\partial_\mu \Sigma \partial_\nu \Sigma^\dagger \partial^\nu \Sigma \partial^\nu \Sigma^\dagger) - \frac{1}{2} \text{Str}(\partial_\mu \Sigma \partial^\nu \Sigma^\dagger)^2 \right. - \text{Str}(\partial_\mu \Sigma \partial_\nu \Sigma^\dagger) \cdot \text{Str}(\partial^\nu \Sigma \partial^\nu \Sigma^\dagger) + 2 \text{Str}(\partial_\mu \Sigma \partial^\nu \Sigma^\dagger \partial_\nu \Sigma \partial^\nu \Sigma^\dagger) \right\}.$$

The operator $O_{PQ}$ should be added to the PQ chiral Lagrangian multiplied by an undetermined coefficient, which we call $L_{PQ}$. This new operator is the subtlety overlooked in Refs. [5, 6].

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5 The fact that this combination vanishes in $SU(3)$ can be most easily seen using the Cayley-Hamilton theorem, as nicely addressed in Ref. [5].

6 To be precise, $O_{PQ}$ vanishes whenever $\Sigma$ has a block-diagonal form with one block, contained entirely within the ungraded $SU(N)$, being an $SU(3)$ matrix, and the other being the identity.
FIG. 3: Scattering process to which $O_{PQ}$ does not contribute. It is physical when $A$ and $B$ are sea quarks, and unphysical when they are valence quarks (with masses differing from those of sea quarks).

FIG. 4: Unphysical scattering process because it involves more than three quarks. Here $A$, $B$, $C$, and $D$ are all different.

III. CONSEQUENCES OF THE NEW OPERATOR AT NLO

We now discuss the consequences of the additional operator. In general, its presence implies that PQ$\chi$PT has an additional NLO coefficient that affects mesonic quantities, and which must be accounted for in lattice fits. Thus it complicates, but does not invalidate, the program of using PQ$\chi$PT to extract the real $\chi$PT coefficients. In particular, since the operator has four derivatives it does not contribute to PGB masses and decay constants, nor to the hairpin vertex of [1], at tree-level. It only contributes to these quantities at one-loop order, which is NNLO in the chiral expansion. We return to these contributions in the next section.

In this section we consider the quantities to which $O_{PQ}$ does contribute at NLO. These are tree-level scattering processes, involving at least four PGBs. We focus on the simplest, four-meson, scattering processes. We illustrate such processes using quark line diagrams, which show the flow of quarks within the mesons. $O_{PQ}$ contains both single and double supertraces, so it contributes to both connected and disconnected quark line diagrams. Here we discuss the types of charged meson scattering processes to which $O_{PQ}$ does and does not contribute.

Because $O_{PQ}$ vanishes in the unquenched $SU(3)$ limit, it cannot contribute at tree-level to scattering processes that occur in the unquenched $SU(3)$ sector. In fact, since the operator has no dependence on the quark mass (i.e. no factors of $\chi$), it cannot distinguish between sea and valence quarks. In other words, its contributions are the same as in the chiral limit, in which limit there is a full $SU(N_{valence} + N_{sea})$ symmetry among quarks. It follows that any scattering process involving three or fewer quarks, whether they are valence or sea quarks, is equivalent to an $SU(3)$ process, and cannot receive a contribution from $O_{PQ}$. One such process is shown in Fig. 3. Mathematically, the contribution of $O_{PQ}$ to this process vanishes because relative minus signs and numbers of Wick contractions among the quark line diagrams produce cancellations. Note that these cancellations would not occur if either or both of the quarks in Fig. 3 were bosonic.

$O_{PQ}$ does contribute to scattering processes that are unique to the PQ theory, and thus unphysical. For example, that shown in Fig. 4 involves four quark flavors. In the case of PQ QCD with $N_{sea} = 3$, these could be four valence quarks, three sea quarks and a valence quark, or other possibilities. Figure 5 is also unique to the PQ theory, involving both valence and ghost quarks. It is clear that $O_{PQ}$ contributes to these processes because there is only one quark-line

7 Quark lines follow the flavor indices of the meson fields within each supertrace.
8 We do not consider processes involving neutral mesons because double poles in the meson propagators make it unclear how to amputate diagrams and thus define scattering amplitudes even at tree level.
diagram and thus no possibility of cancellations. These examples illustrate the origin of the additional operator: the extra particles present in the PQ theory allow the separation of individual quark contractions in a way not possible in the unquenched sector. The same explanation holds for physical theories with four or more flavors.

These unphysical scattering processes can be used, in principle, to determine $L_{PQ}$, the coefficient of the new operator in the PQ chiral Lagrangian. To illustrate this we have calculated some representative scattering amplitudes. First, we give the expression for the “physical” process of Fig. 3.

$$M_3 = \frac{32}{f^4} L_1 \left[ (p_1 \cdot p_3)(p_2 \cdot p_4) + (p_1 \cdot p_2)(p_3 \cdot p_4) \right]$$

$$- \frac{16}{f^4} L_2 \left[ (p_1 \cdot p_2)(p_3 \cdot p_4) + (p_1 \cdot p_3)(p_2 \cdot p_4) + 2(p_1 \cdot p_4)(p_2 \cdot p_3) \right]$$

$$- \frac{16}{f^4} L_3 \left[ (p_1 \cdot p_2)(p_3 \cdot p_4) + (p_1 \cdot p_3)(p_2 \cdot p_4) \right]$$

$$- \frac{16}{f^4} L_4 m_{AB}^2 \left[ (p_1 \cdot p_3)(p_2 \cdot p_4) - (p_1 \cdot p_2)(p_3 \cdot p_4) \right]$$

$$- \frac{4}{f^4} L_5 m_{AB}^2 \left[ (p_1 \cdot p_3)(p_2 \cdot p_4) - (p_1 \cdot p_2)(p_3 \cdot p_4) \right]$$

$$- \frac{64}{f^4} L_6 m_{AB}^4 - \frac{32}{f^4} L_6 \left( \sum_{\text{sea}} \chi_{\text{sea}} \right) m_{AB}^2 - \frac{128}{f^4} L_6 m_{AB}^4$$

(21)

where the momenta are Euclidean and are defined in the figure, and $m_{AB}$ is the leading order mass as given in Eq. 9. Note that, as claimed above, the amplitude does not contain a term proportional to $L_{PQ}$. This is true even though the process may involve only valence quarks with masses differing from those of sea quarks, and thus be unphysical.

The unphysical processes in Figs. 4 and 5 are chosen so that they only receive contributions from disconnected quark line diagrams. It follows that their scattering amplitudes only receive contributions from double supertrace operators, and both have terms proportional to $L_{PQ}$. The amplitude for Fig. 4 is

$$M_4 = \frac{32}{f^4} L_1 (p_1 \cdot p_3)(p_2 \cdot p_4) - \frac{16}{f^4} L_{PQ} \left[ (p_1 \cdot p_2)(p_3 \cdot p_4) + (p_1 \cdot p_3)(p_2 \cdot p_4) + (p_1 \cdot p_4)(p_2 \cdot p_3) \right]$$

$$- \frac{16}{f^4} L_4 \left[ m_{CD}^2 (p_1 \cdot p_3 + p_1 \cdot p_4) + m_{CD}^2 (p_2 \cdot p_3 + p_2 \cdot p_4) \right] - \frac{32}{f^4} L_6 m_{AB}^2 m_{CD}^2,$$

$$- \frac{32}{f^4} L_6 \left( \sum_{\text{sea}} \chi_{\text{sea}} \right) \frac{m_{AB}^2 + m_{CD}^2}{2}$$

(22)

The amplitude for Fig. 5 is really a special case of Eq. 22, obtained by setting $\chi_{C} = \chi_{A}$ and $\chi_{D} = \chi_{B}$, and including an overall sign because Fig. 5 contains one pair of bosonic quarks, and therefore one supertrace over bosonic indices. The kinematic factors are identical because the quark line diagrams have the same structure.

These amplitudes provide a method, in principle, of determining $L_{PQ}$ from PQ simulations. The idea is to calculate the scattering amplitudes, as a function of the valence masses and momenta, and thus determine $L_{1-3}$ from $M_3$ ($L_{4,5,6,8}$ having been obtained from fits to the PGB masses at NLO [1, 2], and then determine $L_{PQ}$ from $M_4$. Other amplitudes involving different external quarks can also be used. In practice, it is not possible to determine the scattering amplitude itself, because the standard method for doing so relies on unitarity [3], and this is violated at the one-loop level in these amplitudes [4, 10]. Instead, what must be done is to use PQχPT to predict the form of Euclidean finite volume correlation functions, which will be given in terms of $L_{PQ}$ and other low energy constants,
and fit this to lattice results for these correlation functions. In this way the unphysical nature of the PQ theory is accounted for.

IV. CONSEQUENCES OF THE NEW OPERATOR AT NNLO

As noted above, $O_{PQ}$ contributes to PGB masses and decay constants first at NNLO in PQQCD. We have calculated these contributions as a first step in extending the application of PQ QCD to this order. To simplify calculations we consider only two valence quarks, $A$ and $B$, and $N$ sea quarks of equal mass. We also only consider the properties of charged mesons, $\pi_{AB}$, figures 6 and 7 show the diagrams contributing to the mass and decay constant of charged mesons. All of the meson diagrams receive contributions from the classes of quark line diagrams shown in figure 8. Quark line diagrams show the effect of partial quenching—valence quarks appear only as external states because ghost quarks cancel them in loops. The series of sea quark hairpin diagrams removes the flavor singlet propagator, enforcing the fact that graded generators are traceless.

The corrections to the renormalized meson mass and decay constant from the new PQ operator (using dimensional regularization and the $\overline{MS}$ scheme of Ref. [11]) are:

$$
\left( \delta m_{AB}^2 \right)_{L_{PQ}} = \left( \frac{\chi_A + \chi_B}{2} \right) \frac{L_{PQ}}{16\pi^2 f^4} \times \left\{ \left( N^2 - 1 \right) \chi_S^2 \left[ \frac{-1}{8} - \frac{3}{2} \ln \chi_S \right] + \left( \frac{\chi_A + \chi_B}{2} \right)^2 \left[ \frac{-1}{4} - 3 \ln \frac{\chi_A + \chi_B}{2\mu^2} \right] \\
+ N \left( \frac{\chi_A + \chi_S}{2} \right)^2 \left[ \frac{1}{4} + 3 \ln \frac{\chi_A + \chi_S}{2\mu^2} \right] + N \left( \frac{\chi_B + \chi_S}{2} \right)^2 \left[ \frac{1}{4} + 3 \ln \frac{\chi_B + \chi_S}{2\mu^2} \right] \\
- \frac{1}{N} \left[ \chi_A^2 \left( \frac{1}{4} + 3 \ln \frac{\chi_A}{\mu^2} \right) + \chi_A \left( \chi_S - \chi_A \right) \left( -2 - 6 \ln \frac{\chi_A}{\mu^2} \right) \right] \\
- \frac{1}{N} \left[ \chi_B^2 \left( \frac{1}{4} + 3 \ln \frac{\chi_B}{\mu^2} \right) + \chi_B \left( \chi_S - \chi_B \right) \left( -2 - 6 \ln \frac{\chi_B}{\mu^2} \right) \right] \\
- \frac{2}{N} \chi_A^2 \left( \frac{\chi_A - \chi_S}{\chi_A - \chi_B} \right) \left( \frac{1}{8} + \frac{3}{2} \ln \frac{\chi_A}{\mu^2} \right) - \frac{2}{N} \chi_B^2 \left( \frac{\chi_B - \chi_S}{\chi_B - \chi_A} \right) \left( \frac{1}{8} + \frac{3}{2} \ln \frac{\chi_B}{\mu^2} \right) \right\} 
$$

(23)

$$
\left( \delta f_{AB} \right)_{L_{PQ}} = \frac{f L_{PQ}}{16\pi^2 f^4} \times \left\{ \left( N^2 - 1 \right) \chi_S^2 \left[ \frac{-1}{16} - \frac{1}{8} \ln \chi_S \right] + \left( \frac{\chi_A + \chi_B}{2} \right)^2 \left[ \frac{-1}{8} - \frac{1}{2} \ln \frac{\chi_A + \chi_B}{2\mu^2} \right] 
$$

9 The simplest example of this is the hairpin correlator discussed in Ref. [1], which is predicted to have a double pole, and thus is manifestly unphysical. Nevertheless, its coefficient, if it can be determined, gives information about physical low energy constants $L_5$ and $L_7$. We note that in the quenched theory, where one also expects a double pole, its coefficient has been successfully determined from fits.
FIG. 8: Quark line diagrams contributing to mass and decay constant renormalization.

FIG. 9: NNLO PGB mass renormalization from operators in $\mathcal{L}_6$

\[
+ N \left( \frac{\chi_A + \chi_S}{2} \right)^2 \left\{ \frac{1}{18} + \frac{1}{2} \ln \left( \frac{\chi_A + \chi_S}{2\mu^2} \right) \right\} + N \left( \frac{\chi_B + \chi_S}{2} \right)^2 \left\{ \frac{1}{18} + \frac{1}{2} \ln \left( \frac{\chi_B + \chi_S}{2\mu^2} \right) \right\}
\]

\[
+ \frac{1}{N} \left[ \chi_A^2 \left( -\frac{1}{8} - \frac{1}{2} \ln \frac{\chi_A}{\mu^2} \right) + \chi_A \left( \chi_S - \chi_A \right) \left( \ln \frac{\chi_A}{\mu^2} \right) \right]
\]

\[
+ \frac{1}{N} \left[ \chi_B^2 \left( -\frac{1}{8} - \frac{1}{2} \ln \frac{\chi_B}{\mu^2} \right) + \chi_B \left( \chi_S - \chi_B \right) \left( \ln \frac{\chi_B}{\mu^2} \right) \right]
\]

\[
+ \frac{1}{N} \chi_A^2 \left( \frac{\chi_A - \chi_S}{\chi_A - \chi_B} \right) \left[ -\frac{1}{8} - \frac{1}{2} \ln \frac{\chi_A}{\mu^2} \right] + \frac{1}{N} \chi_B^2 \left( \frac{\chi_B - \chi_S}{\chi_B - \chi_A} \right) \left[ -\frac{1}{8} - \frac{1}{2} \ln \frac{\chi_B}{\mu^2} \right]
\]

where $\mu$ is the renormalization scale. It can be seen that the corrections in Eqs. 23 and 24 are NNLO by the fact that they have the form $\chi^2 \ln(\chi)$. A check of these results is that if $A$ and $B$ are sea quarks, and if $N_{\text{sea}} = 3$, the mesons in Figs. 6 and 7 live in the unquenched $SU(3)$ sector and cannot get contributions from $O_{\text{PQ}}$. Equations 23 and 24 do, in fact, vanish in the unquenched limit: $\chi_A = \chi_B = \chi_S$, $N_{\text{sea}} = 3$.

We stress that these results are only part of the NNLO charged meson mass and decay constant corrections. The full correction receives 2-loop contributions from $\mathcal{L}_2$, 1-loop contributions from terms in $\mathcal{L}_4$ other than $O_{\text{PQ}}$, and tree-level contributions from $\mathcal{L}_6$. We next discuss the contributions from $\mathcal{L}_6$.

V. ANALYTIC NNLO MASS AND DECAY CONSTANT CORRECTIONS

Fits of present PQ lattice data require NNLO terms [12, 13, 14]. Full non-analytic NNLO calculations in PQ$\chi$PT are not available, so, as an intermediate step, we have determined the form of the analytic NNLO mass and decay constant corrections for charged mesons. These arise from the tree-level diagram in Fig. 9.

This diagram gets contributions from operators in $\mathcal{L}_6$ with zero and two derivatives. Analytic, NNLO decay constant corrections come from a similar diagram, but with an axial current insertion, and only come from two-derivative operators. As in the case of $O_{\text{PQ}}$, we need to be sure to include all operators in the PQ theory, some of which may be linearly-dependent in unquenched $SU(3)$.

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10 The same holds true for $N_{\text{sea}} = 2$, where $O_{\text{PQ}}$ also vanishes.
First we determine the number of linearly-independent, derivative-free operators in $\mathcal{L}_6$. As always, these must be invariant under chiral symmetry transformations, hermitian, and invariant under the discrete symmetries respected by QCD: C, P, and T. They must have three $\chi$ matrices to be $\mathcal{O}(\epsilon^6)$. It is easy to construct terms with the correct symmetry properties using the following two building blocks with simple transformation properties:

$$
\chi^{\dagger} \Sigma \rightarrow (R \chi^{\dagger} L^{\dagger})(LU R^{\dagger}) = R(\chi^{\dagger} \Sigma)R^{\dagger}
$$

$$
\Sigma^{\dagger} \chi \rightarrow (R \chi^{\dagger} L^{\dagger})(L \chi R^{\dagger}) = R(\Sigma^{\dagger} \chi)R^{\dagger}
$$

We find seven allowed forms:

1. \((\text{Str}(\chi^{\dagger} \Sigma))^3 + (\text{Str}(\Sigma^{\dagger} \chi))^3\)
2. \(\text{Str}(\chi^{\dagger} \Sigma \chi \Sigma^{\dagger} \Sigma) + \text{Str}(\Sigma^{\dagger} \chi \Sigma^{\dagger} \Sigma \chi)\)
3. \(\text{Str}(\chi^{\dagger} \Sigma \chi \Sigma^{\dagger} \Sigma) \text{Str}(\chi^{\dagger} \Sigma) + \text{Str}(\Sigma^{\dagger} \chi \Sigma^{\dagger} \Sigma) \text{Str}(\Sigma^{\dagger} \chi)\)
4. \(\text{Str}(\chi^{\dagger} \Sigma \Sigma^{\dagger} \Sigma) \text{Str}(\Sigma^{\dagger} \chi) + \text{Str}(\Sigma^{\dagger} \chi \Sigma^{\dagger} \Sigma) \text{Str}(\Sigma^{\dagger} \chi)\)
5. \(\text{Str}(\chi^{\dagger} \Sigma)^2 \text{Str}(\Sigma^{\dagger} \chi) + (\text{Str}(\Sigma^{\dagger} \chi))^2 \text{Str}(\chi^{\dagger} \Sigma)\)
6. \(\text{Str}(\chi^{\dagger} \Sigma \Sigma^{\dagger} \Sigma) \text{Str}(\chi^{\dagger} \Sigma) + \text{Str}(\chi^{\dagger} \Sigma \Sigma^{\dagger} \Sigma) \text{Str}(\Sigma^{\dagger} \chi)\)
7. \(\text{Str}(\chi^{\dagger} \Sigma \Sigma^{\dagger} \Sigma) \text{Str}(\Sigma^{\dagger} \chi) + \text{Str}(\Sigma^{\dagger} \chi \Sigma^{\dagger} \Sigma) \text{Str}(\Sigma^{\dagger} \chi)\)

(The last two can be simplified using $\Sigma^{\dagger} \Sigma = 1$, but we choose not to do so to better show their form.) Our task is to reduce them to a linearly independent set using group-specific relations.

For $SU(3)$ we can use the Cayley-Hamilton theorem, which states that any matrix satisfies its own characteristic equation, and gives rise to numerous relations between traces of matrices. The relevant relation here is that the determinant of a matrix can be expressed as a polynomial in traces of the matrix of order the size of the matrix. For $3 \times 3$ matrices, this polynomial is

\[
\det(M) = \frac{1}{3} \text{Tr}(M^3) - \frac{1}{2} \text{Tr}(M^2) \text{Tr}(M) + \frac{1}{6} \left( \text{Tr}(M)^3 \right)
\]

Since $\det(\chi^{\dagger} \Sigma) = \det(\chi)^3 = \text{const.}$, the first three operators in the list are linearly dependent. Thus there are only six independent derivative-free $\mathcal{O}(\epsilon^6)$ operators in $SU(3)$.

There is no analogous relationship among operators in the PQ theory, because the super-determinant is not a finite polynomial. The same holds true for $SU(N)$, $N \geq 4$, since the Cayley-Hamilton relations involve quartic or higher-order polynomials, and do not imply any linear dependence among third order polynomials. We conclude there are seven derivative-free operators in PQ$\chi$PT, and also in unquenched $SU(N)$ theories with $N \geq 4$. One of the seven PQ operators can be chosen to be unphysical, namely the linear combination given in Eq. (26) with trace replaced with supertrace. While our PQ result is new, we note that Ref. [15] enumerates all of the operators in the $\mathcal{O}(\epsilon^6)$ chiral Lagrangian for unquenched $SU(N)$. Ref. [16] lists seven linearly-independent operators in $SU(N)$, $N \geq 4$, and six in $SU(3)$, so our results our consistent.

For terms involving two derivatives, we can use group theory to determine the number of independent operators, generalizing the method used earlier in Sec. [11]. To be $\mathcal{O}(\epsilon^6)$ such operators must also contain two factors of $\chi$. We construct these operators using right-handed Lie derivatives and the matrices defined in Eq. (26), all of which transform non-trivially only under the right-handed chiral group. We recall from Sec. [11] that the Lie derivative transforms like an adjoint, so an operator with two Lie derivatives (which are necessarily contracted together by Lorentz symmetry) must be symmetric in this pair of adjoints. The symmetric product of two adjoints is shown in Fig. 2. $\Sigma^{\dagger} \chi$ and $\chi^{\dagger} \Sigma$ transform as bi-fundamentals under the chiral symmetry group, but are not traceless, and so contain both adjoint and singlet parts. Therefore any operator that contains two of these matrices also comes from the product of an adjoint plus singlet times an adjoint plus singlet, as shown in Fig. [10]. If the operator contains two of the same matrices (either $\Sigma^{\dagger} \chi$ or $\chi^{\dagger} \Sigma$), it will only come from the symmetric part of this product, shown in Fig. [11]. Putting this together, we must construct singlets out of the product in Fig. 2 which comes from the Lie derivatives, and that in either Fig. [10] or [11] which come from the terms involving factors of $\chi$.

In this way, we find that eight linearly-independent operators can be made out of two Lie derivatives, one $\Sigma^{\dagger} \chi$, and one $\chi^{\dagger} \Sigma$. They correspond to the eight flavor singlets $\Sigma$ in the direct product of the representations in Figs. 2 and 11. One choice of basis is the following,

1. $\text{Str}(\partial_\mu \Sigma^{\dagger} \partial_\mu \Sigma \chi^{\dagger} \chi)$
\[
(\begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + 1) \times (\begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + 1) = \left( \begin{array}{c}
\bullet \bullet \bullet \\
\bullet \bullet \bullet \\
\end{array} + \begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + \\
\begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + \begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + \\
\begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + 1 \right) \\
+ \left( \begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + \begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} \right) + 1
\]

FIG. 10: The product of two bi-fundamentals in SU(N|M). The result also applies for SU(N) for N > 3 (with the dashed lines removed).

\[
\left[ \begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + 1 \right] \times \left[ \begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + 1 \right] = \left( \begin{array}{c}
\bullet \bullet \bullet \\
\bullet \bullet \bullet \\
\end{array} + \\
\begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + \\
\begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} + 1 \right) + \left( \begin{array}{c}
\bullet \bullet \\
\bullet \bullet \\
\end{array} \right) + 1
\]

FIG. 11: Symmetric product of two bi-fundamentals in SU(N|M). The result also applies to SU(N) for N > 3 (with the dashed lines removed).

2. \(\text{Str}(\partial_{\mu} \Sigma^I \chi^I \partial_{\mu} \Sigma)\)
3. \(\text{Str}(\partial_{\mu} \Sigma^I \chi^I \partial_{\mu} \Sigma \chi^I \Sigma)\)
4. \(\text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma) \text{Str}(\chi^I \chi)\)
5. \(\text{Str}(\partial_{\mu} \Sigma^I \chi) \text{Str}(\chi^I \Sigma)\)
6. \(\text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma \text{Str}(\chi^I \Sigma) \text{Str}(\Sigma^I \chi))\)
7. \(\text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma \chi^I \Sigma) \text{Str}(\Sigma^I \chi)\)
8. \(\text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma \Sigma^I \chi) \text{Str}(\chi^I \Sigma)\)

where the derivatives act only on the quantity immediately to their right, and we have used the anti-Hermiticity of the Lie derivatives to simplify some of the operators. Although group theory gives operators with the right chiral transformation properties, we must impose the other symmetries by hand. Operators 1 and 2 transform into each other under parity, so we must include their sum, with a single coefficient, in the Lagrangian. Operators 7 and 8 are hermitian conjugates, so we must include their sum as a single operator as well. We conclude that there are six operators of the above type in the PQ chiral Lagrangian.

Similarly, six operators can be made out of two Lie derivatives and two \(\Sigma^I \chi^I s\) or \(\chi^I \Sigma s\) because there are two fewer adjoints in the symmetric product of Fig. 11.

1. \(\text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma \chi^I \Sigma + \partial_{\mu} \Sigma^I \partial_{\mu} \Sigma \Sigma^I \chi^I \Sigma)\)
2. \(\text{Str}(\partial_{\mu} \Sigma^I \chi \partial_{\mu} \Sigma^I \chi + \chi^I \partial_{\mu} \Sigma \chi^I \partial_{\mu} \Sigma)\)
3. \(\text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma) \text{Str}(\chi^I \Sigma^I \chi + \Sigma^I \chi \Sigma^I \chi)\)
4. \(\text{Str}(\chi^I \partial_{\mu} \Sigma) \text{Str}(\chi^I \partial_{\mu} \Sigma) + \text{Str}(\partial_{\mu} \Sigma^I \chi) \text{Str}(\partial_{\mu} \Sigma^I \chi)\)
5. \(\text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma \chi^I \Sigma) \text{Str}(\chi^I \Sigma) + \text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma \Sigma^I \chi) \text{Str}(\Sigma^I \chi)\)
6. \(\text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma) \text{Str}(\chi^I \Sigma) \text{Str}(\chi^I \Sigma) + \text{Str}(\partial_{\mu} \Sigma^I \partial_{\mu} \Sigma) \text{Str}(\Sigma^I \chi) \text{Str}(\Sigma^I \chi)\)

This completes the counting for the PQ theory: there are twelve linearly independent two-derivative operators in \(\mathcal{L}_6\). The same result applies to SU(N) for N > 3. For SU(3), however, one operator can be eliminated from each of the two previous lists in because there is one fewer representation in the product of adjoints for SU(3) than for SU(N|M). We can use Cayley-Hamilton relations analogous to Eq. (26) to obtain the precise relationship between
the operators. Thus there are only ten two-derivative operators in \(SU(3)\), and correspondingly two unphysical operators in the PQ theory. Our results for \(SU(N)\) are consistent with those of Ref. 15.

We stress that the counting of operators in all \(SU(N|M)\) PQ theories is valid for any \(N > M \geq 2\). The superdeterminant is not a finite polynomial in any such theory, and there are no Cayley-Hamilton relations. From the perspective of Young tableaux, this result follows because the theories do not have an antisymmetric tensor to contract indices, and in particular there is no limit to the number of boxes in the column of a Young tableau, as there is in \(SU(N)\).

We now return to the NNLO corrections to the PGB mass and decay constant. Although there are contributions from all of the operators in \(\mathcal{L}_6\) enumerated above, the form of the tree-level correction to the mass of \(\pi_{AB}\) is simple: 12

\[
\left(\frac{\delta m_{AB}^2}{m_{AB}^2}\right)_{N^{NLO}, \text{Analytic}} = \alpha_1 \text{tr}(\chi_S^2) + \alpha_2 \text{tr}(\chi_S^2)^2 + \alpha_3 \text{tr}(\chi_S^2)\left(\chi_A + \chi_B\right) + \alpha_4 \left(\chi_A + \chi_B\right)^2 + \alpha_5 \left(\chi_A - \chi_B\right)^2.
\] (27)

Here \(\chi_S\) is the mass matrix of the sea quarks. In fact, Eq. (27) is the most general quadratic polynomial separately symmetric in the valence and sea quark masses. The \(\alpha_i\) are linear combinations of \(\mathcal{L}_6\) coefficients, and we have checked that they are independent, so that no relations are predicted among the \(\alpha_i\). Corrections to \(f_{AB}\) have the same form with different coefficients. Fits in Ref. 15 to PQ lattice data with \(\frac{4}{3}m_S < m_{\text{sea}} < \frac{2}{3}m_S\) are consistent with this NNLO formula.

It is interesting to consider the contributions to the \(\alpha_i\) from the three unphysical operators. We find that these operators do contribute to the \(\alpha_i\) (in fact, to all five of them in the basis we use), i.e., that the unphysical operators affect PGB properties at tree level. 13 This is different from \(\mathcal{O}_{PQ}\), which does not affect PGB properties until one-loop order. It implies that the \(\alpha_i\) are linear combinations of the coefficients of physical and unphysical operators. Clearly, since the number of low energy constants entering at NNLO (nineteen in the zero and two-derivative sector alone) exceeds the number of constraints from PGB masses and decay constants (ten in the PQ theory 14), one must use other quantities in order to completely determine all the constants.

Just as at NLO 13, using the PQ theory can simplify this determination. Consider the case of degenerate sea quarks. The unquenched sector alone constrains only two combinations of constants (one each from the single term proportional to \(\chi_A^2 = \chi_B^2 = \chi_S^2\) in \(\delta m_{AB}^2\) and \(\delta f_{AB}\)), although these combinations necessarily involve only physical constants. Consideration of the PQ theory adds three unphysical operators, but this “cost” is outweighed by the benefit of the six additional constraints from Eq. (27). 15 In addition, using the PQ theory one can add more values of \(\chi_A\) and \(\chi_B\) to the fit at relatively small computational expense.

If one uses non-degenerate sea quarks then only the second benefit of partial quenching applies. This is because, even in the unquenched sector, one can, in principle, determine four of the five \(\alpha_i\) for both PGB masses and decay-constants, using a number of choices for the sea quark masses. 16 Moving to the PQ theory gives two more constraints but at the cost of three unphysical operators. Nevertheless, we suspect that this cost will be easily outweighed by the additional data points that one can obtain in the PQ theory.

VI. CONCLUSION

In this paper we have discussed a complication to the program of using simulations of unphysical PQ theories to obtain physical low energy constants. We find that there are operators in PQ\(\chi\)PT which vanish when restricted to the physical, unquenched sector of the theory. There is one such unphysical operator in the NLO Lagrangian \(\mathcal{L}_4\), and three in the zero and two derivative part of \(\mathcal{L}_6\). Generically, we expect the number of unphysical operators to increase with the order of the calculation. Their presence is related to the fact that correlation functions in the

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11 See Ref. 5 for details.
12 This result has also been obtained independently by Ref. 14.
13 Of course, by definition, the total contribution of unphysical operators to \(\delta m_{AB}^2\) must vanish when both \(\chi_A\) and \(\chi_B\) are equal to sea quark masses, and we have checked this explicitly for the combination appearing in Eq. (26) with \(N_{\text{sea}} = 3\).
14 There are five each from Eq. (27) and the analogous expression for \(\delta f_{AB}\).
15 There are three each from \(\delta m_{AB}^2\) and \(\delta f_{AB}\), rather than four, because the first two terms collapse into a single term for degenerate sea quarks.
16 With three sea quarks there are four independent quadratic combinations of masses that are symmetric under \(A \leftrightarrow B\): \((\chi_A \pm \chi_B)^2\), \(\chi_C^2\), and \((\chi_A + \chi_B)\chi_C\).
The unquenched sector involve linear combinations of quark contractions, while in the larger PQ theory one can determine each contraction separately.

Dealing with this complication is, in principle, straightforward. The contributions from unphysical operators can be disentangled from those of physical operators as long as one considers enough quantities in the fits. The extent of this complication will depend on the example being considered. For the quantities we have studied in detail, the PGB masses and decay constants, the new $\mathcal{O}(p^4)$ operator $\mathcal{O}_{PQ}$ does not contribute at tree level to PGB masses and decay constants, and so one does not need to include it at all until one works at NNLO.

As a case study in how to deal with the complication of unphysical operators, we have outlined a strategy for how one could, in principle, determine and subtract the NNLO contributions of $\mathcal{O}_{PQ}$ to PGB properties. Our idea is to determine its coefficient using unphysical scattering processes, to which $\mathcal{O}_{PQ}$ contributes at the first non-vanishing order, which is NLO in $\chi$PT. Then, when doing a NNLO fit to the PGB properties, one can subtract the contribution from $\mathcal{O}_{PQ}$, the form of which we have calculated. Of course, any such fit would require all other NNLO terms, including two-loop contributions with vertices from $\mathcal{L}_2$, and these are not yet available for the PQ theory.

We have also considered the more difficult question of how to separate the contributions from the unphysical operators in $\mathcal{L}_6$. The difference here is that these operators contribute to PGB masses and decay constants at tree level, so their coefficients appear in combination with those of the physical NNLO operators. One must therefore rely on the general strategy of calculating enough quantities to constrain all the coefficients, both physical and unphysical.

Clearly, extending the determination of low energy constants to NNLO in the meson sector is a significant undertaking, requiring extensive $\chi$PT calculations beyond those presently available, and consideration of many quantities in addition to PGB masses and decay constants. If such a program is undertaken, PQ simulations can play an important role. While they introduce a few additional unknown constants, they provide both additional constraints on low energy constants from the extra functions of valence masses that are available, and, most importantly, the possibility of additional, relatively cheap, data points to include in the fits.

Finally, we take this opportunity to reiterate the purpose of simulating PQ QCD. The intent is not to study it as an approximation to, or a model of, QCD, for it is an unphysical theory, but rather to use it as a tool to more easily extract the low energy constants of QCD. Once these are determined, they can be used to calculate PGB processes in QCD, including those that are not easily accessible to lattice calculations. The unphysical nature of PQ QCD is manifested in several ways, for example by the presence of double poles in neutral propagators, and by the inability to define decay and scattering amplitudes. We have discussed here another unphysical feature, namely the presence of additional operators in PQ$\chi$PT which do not contribute in the unquenched sector. While all these features do complicate the use of PQ QCD, we have argued that these complications can be overcome and that PQ simulations remain an important element of the lattice practitioner’s toolkit.

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