Partially quenched chiral perturbation theory without Φ_0

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This paper completes the argument that lattice simulations of partially quenched QCD can provide quantitative information about QCD itself, with the aid of partially quenched chiral perturbation theory. A barrier to doing this has been the inclusion of Φ_0, the partially quenched generalization of the η', in previous calculations in the partially quenched effective theory. This invalidates the low energy perturbative expansion, gives rise to many new unknown parameters, and makes it impossible to reliably calculate the relation between the partially quenched theory and low energy QCD. We show that it is straightforward and natural to formulate partially quenched chiral perturbation theory without Φ_0, and that the resulting theory contains the effective theory for QCD without the η'. We also show that previous results, obtained including Φ_0, can be reinterpreted as applying to the theory without Φ_0. We contrast the situation with that in the quenched effective theory, where we explain why it is necessary to include Φ_0. We also compare the derivation of chiral perturbation theory in partially quenched QCD with the standard derivation in unquenched QCD. We find that the former cannot be justified as rigorously as the latter, because of the absence of a physical Hilbert space. Finally, we present an encouraging result: unphysical double poles in certain correlation functions in partially quenched chiral perturbation theory can be shown to be a property of the underlying theory, given only the symmetries and some plausible assumptions.

I. INTRODUCTION

Numerical simulations of lattice QCD are hampered by the difficulty of including loops of light quarks. This has forced the use of approximations to the fermion determinant: the quenched approximation (setting the determinant to a constant), and, more recently, the partially quenched (PQ) approximation (including the determinant but with sea quark masses different from, and typically larger than, those of the valence quarks). While all such simulations correspond to unphysical theories, they are not all equally unphysical. It has been argued recently that PQ simulations can be used to obtain physical parameters if the quarks are light enough that one can use chiral perturbation theory to describe the low energy properties of the theory [1–3]. The only approximation necessary is the truncation of chiral perturbation theory. On the other hand, if the sea quarks are too heavy, then partial quenching is an uncontrolled approximation whose results will at best be a qualitative guide to those in the physical theory.

The main purpose of this paper is to complete the theoretical argument justifying the use of PQ simulations to obtain physical parameters. The missing ingredient in the arguments presented in Refs. [1,3] concerns the flavor-singlet field, Φ_0, which is the generalization of the η' in PQ theories. This field must be kept in the low-energy effective theory for quenched QCD, because its correlation functions contain poles at the masses of the light pseudo-Goldstone mesons. The same holds true for the PQ theory with heavy sea quarks. The need to include Φ_0 invalidates the standard chiral power counting and introduces additional coupling

constants in the chiral Lagrangian. Consequently, progress with this theory can only be made by making further assumptions.

On the other hand, in QCD the η' is not a pseudo Goldstone boson, the corresponding field need not be included in the chiral Lagrangian, and chiral perturbation theory can be developed as a low energy expansion [4–6]. What we demonstrate here is that the situation is similar for PQ QCD with sea (and valence) quarks in the chiral regime: It can be described by a chiral Lagrangian in which Φ_0 is absent, and for which standard power-counting applies. As stressed in Refs. [1,3], an important corollary is that the parameters of the PQ chiral Lagrangian are the same as those in the chiral Lagrangian for QCD. This is what is needed to show that PQ simulations can be used to extract physical parameters.

Another result shown here is of a more technical nature. All previous calculations using PQ chiral perturbation theory have included the Φ_0 field, and thus suffer from the problems described above. Here we show that these problems can be avoided by sending the Φ_0 mass parameter, m_0, to infinity, because this is mathematically equivalent to considering the theory in which Φ_0 is absent. In this way, the results of the previous calculations from PQ chiral perturbation theory can be reinterpreted as applying to the theory for which the matching to QCD is immediate. This observation also justifies the *ad hoc* prescriptions for integrating out Φ_0 that were used previously [7–9,3].

A secondary purpose of this paper is to discuss the theoretical foundations of chiral perturbation theory for PQ theories, building on the work of [10,11]. We recall the line of reasoning used to construct the chiral Lagrangian for QCD, examine the extent to which it applies also to PQ QCD, and point out the gaps that make PQ chiral perturbation theory stand on less secure grounds. We are able to show, however, that a signature prediction of PQ chiral effective theories,

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namely the presence of double pole contributions to flavor singlet correlators, can be derived in the underlying theory from the assumption that valence flavor non-singlet correlators have single poles. The latter assumption is well tested by numerical simulations.

This paper is organized as follows. In the next section we review the definition of PQ theories, and discuss their symmetries. The set of two-point functions containing light poles is identified in Sec. III for both PQ and quenched theories. In Sec. IV we construct the PQ effective Lagrangian that reproduces the previously determined pole structure, and discuss its theoretical foundations. In Sec. V we explain how chiral perturbation theory including Φ_0 is equivalent to that excluding Φ_0 if one sends $m_0 \to \infty$. We then discuss the pole structure of flavor-singlet correlators in Sec. VI, and summarize our conclusions in Sec. VII.

Five Appendixes contain technical details. Appendix A describes the true symmetries of the PQ QCD partition function, derives the resulting Ward identities, and shows how these are in fact the same as those obtained assuming a "fake" symmetry group. Appendix B collects useful results on the diagonal generators of graded Lie groups. Appendix C gives an alternative argument for why one does not need to include Φ_0 in PQ chiral perturbation theory. Appendix D concerns a useful result about the limit $m_0 \to \infty$. Finally, Appendix E derives the constraints on neutral pion correlators using graded symmetries.

II. PARTIALLY QUENCHED THEORIES AND THEIR SYMMETRIES

We consider a theory with N sea quarks and N_V valence quarks, which is viewed as a tool to study an unquenched theory with N quarks. We will shortly consider all quarks, sea and valence, to be light, although this is not needed to set up the definition of the theory. Clearly, the theories we have in mind are those with $N=2$ (treating only the up and down quarks as light) and $N=3$ (also including the strange quark—whose status as a light quark is less clear). The number of valence quarks one usually uses is $N_V=2$ (needed to discuss simple meson properties), or $N_V=3$ (needed for baryon properties).

In practice, one obtains PQ results by generating gauge configurations including in the weight a determinant representing the effect of N sea quarks, and then calculating quark propagators on these background gauge fields using masses which are different from those of the sea quarks. This can be represented theoretically by Morel's construction involving bosonic spin-1/2 ghost fields [12], in which the Euclidean partition function is

$$Z = \int D[\psi \bar{\psi} \tilde{\psi} \bar{\tilde{\psi}} A] \exp\left(-S_G - \int [\bar{\psi}(\slashed{D}+m)\psi \right.$$

$$\left. + \bar{\tilde{\psi}}(\slashed{D}+\tilde{m})\tilde{\psi}] \right)$$

$$= \int D[A] \exp(-S_G) \frac{\det(\slashed{D}+m)}{\det(\slashed{D}+\tilde{m})}. \tag{1}$$

Here S_G is the gauge action, ψ an (N_V+N)-dimensional column vector containing the quark fields, with mass matrix m, and $\tilde{\psi}$ an N_V-dimensional vector of ghost quarks, with mass matrix $\tilde{m}$. For each valence quark there is a ghost quark with the same mass, so that the valence quark determinant cancels precisely against that from the ghost quarks. The complete mass matrix is

$$M = \begin{pmatrix} m & 0 \\ 0 & \tilde{m} \end{pmatrix}$$

$$= \operatorname{diag}(m_{V1}, \dots, m_{VN_V}; m_{S1}, \dots, m_{SN}; m_{V1}, \dots, m_{VN_V}). \tag{2}$$

In the following, we will take all non-zero entries of M to be real and positive.

Our discussion will concern the theory obtained in the continuum limit of PQ simulations. This allows us to take $\slashed{D}$ as having standard continuum properties: it is an anti-Hermitian operator which connects left-handed fields to right-handed fields and vice versa. In this way we avoid the issue of how best to discretize fermions, and of possible difficulties in simulating odd numbers of dynamical quarks. We simply assume that these difficulties have been overcome, and that the lattice simulations are done close enough to the continuum limit that Eq. (1) represents them up to small corrections, suppressed by powers of the lattice spacing, which can be extrapolated away.[1] Indeed by using overlap fermions, or other fermions with an exact chiral symmetry, one can presumably formulate the discussion of symmetries at non-zero lattice spacing.

Correlation functions of quark and ghost fields are defined, as usual, by introducing source terms into Z. Note that if one considers correlation functions involving only sea-quark fields, one obtains exactly the result of the unquenched theory with N sea quarks, because the valence and ghost determinants cancel [10]. Furthermore, if one of the valence quarks has the same mass as a sea quark, then it can replace that sea quark in correlation functions without changing the result [10].

To discuss symmetries, it is useful to collect quarks and ghost quarks into a single $(N+2N_V)$-dimensional vector, Q, defined by

$$Q^T = (\psi^T, \tilde{\psi}^T). \tag{3}$$

The fermionic part of the action then takes the standard form

$$S_F = \int \bar{Q}(\slashed{D}+M)Q$$

$$= \int (\bar{Q}_L \slashed{D} Q_L + \bar{Q}_R \slashed{D} Q_R + \bar{Q}_R M Q_L + \bar{Q}_L M Q_R), \tag{4}$$

where the projections are defined by

$$Q_{L,R} = \frac{(1 \pm \gamma_5)}{2} Q, \quad \bar{Q}_{L,R} = \bar{Q} \frac{(1 \mp \gamma_5)}{2}. \quad (5)$$

The symmetry group of the action Eq. (4), when $M \to 0$, appears to be the graded group

$$U(N_V + N | N_V)_L \otimes U(N_V + N | N_V)_R, \quad (6)$$

under which the fields transform in the usual way

$$Q_{L,R}(x) \to U_{L,R} Q_{L,R}(x), \quad \bar{Q}_{L,R}(x) \to \bar{Q}_{L,R}(x) U_{L,R}^\dagger, \quad (7)$$

with $U_{L,R} \in U(N_V + N | N_V)$. As noted in Ref. [11], however, this is not the correct symmetry because the functional integral over the bosonic spin-1/2 fields converges only if they are properly constrained (and if the mass matrix is positive definite). As a result of the constraint, right- and left-handed fields cannot be rotated independently in the usual way. Nevertheless, it turns out that one can proceed as if the symmetry group were (6), as long as one only considers small transformations. This is explained in Appendix A. In particular we show that one obtains the correct vector and axial Ward identities if one pretends that the action has the symmetry group Eq. (6), rather than the actual symmetry group. In what follows we mostly use the "fake" symmetries, since this emphasizes the similarities to the development for unquenched QCD, and is usually simpler. We use the real symmetries only when global aspects of the symmetry group are important.

Certain of the transformations in Eq. (7) are anomalous, since they do not leave the measure invariant. Removing these requires that we impose the constraint

$$\text{sdet } U_L = \text{sdet } U_R, \quad (8)$$

where "sdet" is the invariant "super-determinant."[2] The overall result is that the chiral symmetry group of the massless PQ theory can be taken to be the group proposed in [10]

$$SU(N_V + N | N_V)_L \otimes SU(N_V + N | N_V)_R \otimes U(1)_V. \quad (10)$$

Here the $U(1)_V$ transformations are common overall phase rotations of the right- and left-handed fields.[3]

The form Eq. (10) reflects the fact that for the PQ case (i.e., $N > 0$), the $U(1)$ factor can be chosen to be a flavor singlet, and thus to commute with all elements of $SU(N_V + N | N_V)$. In particular, the anomalous symmetry current can be chosen to be the flavor singlet, $j_{A\mu}^{(I)} = \bar{Q} \gamma_\mu \gamma_5 Q$ [using the

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[2] Here the super-determinent is defined by $\text{sdet } U = \exp \text{str} \ln U$, with the supertrace being

$$\text{str} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \text{tr } A - \text{tr } D, \quad (9)$$

the blocks corresponding to the $N_V + N$ quark and N_V ghost coordinates, respectively.

[3] We are ignoring the fact that globally $U(N_V + N | N_V) = [SU(N_V + N | N_V) \otimes U(1)]/Z_N$, i.e., it is a coset rather than a direct product. This is irrelevant for small transformations.

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notation of Appendix A, Eq. (A31)]. This has the same quantum numbers as the pseudoscalar density $\bar{Q} \gamma_5 Q$, which is the interpolating field associated with Φ_0 [10]—the focus of much of the subsequent discussion.

The symmetry structure is different for the fully quenched theory, $N = 0$. In particular, as noted in Ref. [13], the flavor singlet $U(1)$ is part of $SU(N_V | N_V)$, while the $U(1)$ with non-unit superdeterminant cannot be chosen to be a flavor singlet, and so does not commute with all elements of $SU(N_V | N_V)$. This is explained more fully in Appendix B, where we collect some results on the generators of graded groups. The net effect is that the $SU(N_V | N_V)$ and $U(1)$ factors form, locally, a semi-direct product, and the chiral symmetry group can be taken to be

$$[SU(N_V | N_V)_L \otimes SU(N_V | N_V)_R] \ltimes U(1)_V. \quad (11)$$

As discussed below, the difference between this group and Eq. (10) is the mathematical result which underlies the need to include the Φ_0 field in the quenched, but not the PQ, chiral Lagrangian.

III. SYMMETRY BREAKING AND THE NEED FOR Φ_0

As could already be seen in the previous section, the introduction of valence and ghost quarks modifies the standard flavor symmetry structure of the theory, and consequently the formulation of the chiral effective theory. One striking example is the non-decoupling of Φ_0 in the fully quenched theory. The main goal of this section is to analyze this phenomenon in some detail, and to demonstrate why it does not carry over to PQ theories. To study this, we investigate which two-point correlation functions contain poles at low energies. In other words, we find the degrees of freedom that one must include in a low energy effective theory for quenched and PQ QCD.

Throughout this section we consider the PQ theory in the chiral limit. This allows us to use the condensate as an order parameter, and to use Goldstone's theorem to determine which channels have massless poles. In the usual way, the chiral limit is to be approached by working at non-zero quark masses and then taking the masses to zero after the volume has been sent to infinity. In the PQ theory there is, however, a subtlety concerning the chiral limit. As noted in Ref. [8], chiral perturbation theory predicts that the PQ theory is singular if one sends valence quark masses to zero with fixed non-zero sea-quark masses. In particular, the condensate itself is singular in this limit. This singularity is similar to that which occurs in the quenched theory [14,13,15]. To avoid this singularity, one should send all the quark masses to zero simultaneously with fixed ratios.[4]

Such a limiting proceedure is not available for the quenched theory. Thus, in the following, when we refer to the quenched theory, we have in mind working close to, but not in, the chiral limit. Since our focus here is on the PQ

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[4] This limiting procedure also avoids divergences from exact zero modes in topologically non-trivial sectors.

theory, we do not revisit the subtleties associated with the quenched chiral limit.

A. Symmetry breaking pattern

As in QCD, we choose the vacuum expectation value (VEV)

$$\Omega_{ab} \equiv \langle \bar{Q}_a Q_b \rangle \tag{12}$$

as an order parameter for chiral spontaneous symmetry breaking.

We first consider the vector symmetries. It was shown long ago by Vafa and Witten that vector symmetries do not spontaneously break in vector-like gauge theories [16]. Their derivation does not make use of Hilbert space states and operators, and relies only on the fact that the quark determinant leads to a real and positive measure in the functional integral over the gauge fields. This is still true for quenched and PQ QCD, and the Vafa-Witten result still holds. Consequently, Ω_{ab} is invariant under vector transformations. It is in fact easier to see what this implies for the related quantity

$$\tilde{\Omega}_{ab} \equiv \langle Q_{b\tau} \bar{Q}_{a\tau} \rangle \tag{13}$$

(τ is a Dirac-color index that must still be contracted to form a Euclidean scalar). This transforms under ("fake") vector transformations in the following way:

$$\tilde{\Omega} \rightarrow V \tilde{\Omega} V^\dagger, \quad V \in SU(N_V + N|N_V). \tag{14}$$

The invariance of Ω under Eq. (14) leads to

$$\tilde{\Omega} = \omega \delta_{ab} \tag{15}$$

where ω is a constant. Interchanging Q and $\bar{Q}$ fields, we obtain

$$\Omega_{ab} = -\omega \delta_{ab} \varepsilon_a \tag{16}$$

where we introduce the notation

$$\varepsilon_a = \begin{cases} 1 & a \text{ is a quark index,} \\ -1 & a \text{ is a ghost index.} \end{cases} \tag{17}$$

The question of whether the axial symmetry is spontaneously broken or not depends on the value of ω. The sea sector of PQ theories is equivalent to unquenched QCD with N quark flavors. An important implication of this fact is that the spontaneous breakdown of axial symmetries in QCD, signaled by the non-vanishing of $\langle \bar{q}q \rangle$, is duplicated in the sea sector of PQ theories, thus implying that $\omega \neq 0$. In other words, given that there is spontaneous chiral symmetry breaking in QCD, the symmetry breaking pattern of PQ QCD is known:[5]

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[5]Here we are assuming $N \geq 2$, since there is no chiral symmetry to break for $N=1$ QCD.

$$SU(N_V+N|N_V)_L \otimes SU(N_V+N|N_V)_R \otimes U(1)_V$$

$$\rightarrow SU(N_V+N|N_V)_V \otimes U(1)_V. \tag{18}$$

This argument does not carry over to the quenched theories, because there is no QCD-like sea sector. For quenched theories the spontaneous breaking of axial symmetries is an additional assumption—though one that is supported by numerical evidence. If we make that assumption, the symmetry breaking pattern for quenched QCD is

$$[SU(N_V|N_V)_L \otimes SU(N_V|N_V)_R] \ltimes U(1)_V$$

$$\rightarrow SU(N_V|N_V)_V \ltimes U(1)_V. \tag{19}$$

B. Low energy poles from symmetries

Once the symmetry breaking pattern has been established, it is a standard result in field theory that the number of pseudo-Goldstone bosons is determined by the number of non-anomalous generators that act non-trivially on the vacuum. For the case at hand one thus expects $(2N_V+N)^2 - 1$ Goldstone particles for PQ theory. Though the group structure in the quenched case is slightly different, the counting argument still gives $(2N_V)^2 - 1$, which is the same expression as for PQ theories with $N=0$. There is, however, a significant difference between the two cases. As the following more careful analysis shows, the simple counting argument correctly predicts the number of Goldstone particles *only* in the PQ case. For the quenched case it turns out that there are $(2N_V)^2$ fields which exhibit long range correlations. The additional field that is needed for quenched QCD is none other than Φ_0.

Consider the two-point correlation function between an axial current $j_{A\mu}^{(T)}(x)$ [defined in Eq. (A31)] and a pseudo-scalar density $\phi^{(T')}(0) = \bar{Q} \gamma_5 T' Q(0)$,

$$C_\mu^{(T,T')}(x) = \langle j_{A\mu}^{(T)}(x) \phi^{(T')}(0) \rangle. \tag{20}$$

Here T and T' label generators of the symmetry group. From Euclidean invariance, its Fourier transform must have the form

$$\tilde{C}_\mu^{(T,T')}(p) = ip_\mu F^{(T,T')}(p^2), \tag{21}$$

where F is an unknown function. Next, consider the Ward identity which follows from applying an infinitesimal axial transformation with generator T to $\langle \phi^{(T')}(0) \rangle$:

$$\partial_\mu C_\mu^{(T,T')}(x) = -\delta(x) \langle \delta_A^{(T)} \phi^{(T')}(0) \rangle \tag{22}$$

[for the definition of $\delta_A^{(T)} \phi$ see Eq. (A32)]. Together, Eqs. (21) and (22) give

$$p^2 F^{(T,T')}(p^2) = -\langle \delta_A^{(T)} \phi^{(T')}(0) \rangle. \tag{23}$$

A straightforward calculation of the right hand side, with the use of the VEV (16), gives

$$p^2 F^{(T,T')}(p^2) = 2\omega str(TT'). \tag{24}$$

(Note that the order of T and T' is important for graded generators.) Equation (24) relies on the fact that T generates a true (non-anomalous) symmetry of the theory. For quenched and PQ theories the non-anomalous symmetries satisfy $str(T) = 0$. Consequently, $\tilde{C}_\mu^{(T,T')}(p)$ has a pole at $p = 0$ for any T and T' for which $str(T) = 0$ and $str(TT') \neq 0$.

It is straightforward to show that, for both quenched and PQ theories, all the flavor off-diagonal ("charged") generators give rise to light poles, like in QCD, and that they do not mix with the neutral ones. Subtleties only arise in the neutral sector, and to study them we use a specific choice of diagonal generators that is presented in Appendix B [Eq. (B7)]. There we find that, for the PQ theory,

$$str(T_a T_b) = \text{diag}(\underbrace{1, \ldots, 1}_{N_V + N - 1}, \underbrace{-1, \ldots, -1}_{N_V - 1}, -1, 1).$$

Here the T_a are diagonal members of the algebra, all straceless but the last one, $T_{2N_V + N} \propto I$, which generates the anomalous $U(1)_A$. Applying Eq. (B7) to Eq. (24) shows that a complete set of (flavor neutral) fields that give rise to long range correlations in two-point functions is

$$\bar{Q} \gamma_5 T_a Q, \quad a = 1, \ldots, 2N_V + N - 1. \tag{25}$$

Note that for N_V of these fields, the coefficient of the massless pole has an unphysical sign, corresponding to the entries with -1 in Eq. (B7). The symmetries do not imply that $\phi^{(T_{2N_V + N})} = \phi^{(I)}/\sqrt{N}$, has a pole at $p = 0$. Consequently, to describe the long distance parts of the two-point functions in the PQ theory we do not need to consider correlators involving the corresponding field, Φ_0.

In the quenched case Eq. (B7) is replaced by

$$str(T_a T_b) = \begin{pmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & -1 & & & & \\ & & & & \ddots & & & \\ & & & & & -1 & & \\ & & & & & & 0 & 1 \\ & & & & & & 1 & 0 \end{pmatrix}.$$

Again, the generator of the anomalous $U(1)_A$ is the last one, $T_{2N_V} \propto \bar{I}$ [defined in Eq. (B6)]. All the other generators are straceless, including $T_{2N_V - 1} = I$. One obtains a new nontrivial equation from Eq. (24) by choosing $T = I$, which is non-anomalous (a fact unique to quenched QCD), and $T' = \bar{I}$. We thus find that the Fourier transform of

$$\langle j_{A\mu}^{(I)}(x) \phi^{(\bar{I})}(0) \rangle \tag{26}$$

has a pole at $p = 0$. Since Φ_0 has the same quantum numbers as

$$j_{A\mu}^{(I)} = \bar{Q} \gamma_\mu \gamma_5 Q \tag{27}$$

we conclude that it must be included in the effective Lagrangian in order to correctly reproduce the low energy behavior of quenched QCD.

Let us summarize why one needs to include Φ_0 in quenched, but not PQ, chiral perturbation theory. A field should be included if either the corresponding pseudoscalar density or axial current can be shown to couple to a Goldstone boson. In unquenched and PQ theories, the argument given above shows that the coupling of a density with flavor generator T implies the coupling of the corresponding current [since $str(T_a T_b)$ is diagonal]. The peculiarity of the quenched theory is that the current with the same quantum numbers as Φ_0, i.e., the flavor singlet $j_{A\mu}^{(I)}$, is *not anomalous* and thus should couple to a Goldstone boson. This is despite the fact that the corresponding density, $\bar{Q} \gamma_5 Q$, is invariant under non-anomalous transformations. Conversely, the anomalous current, $j_{A\mu}^{(\bar{I})}$, is *not a flavor singlet*, and so, as shown above, the corresponding density couples to a Goldstone boson, contrary to naive expectation. Mathematically, this peculiarity is due to the fact that $str(I) = 0$, which leads both to the key result that $str(T_a T_b)$ is not diagonal, and to the semi-direct product structure of the quenched symmetry group, Eq. (11). This is the sense in which the symmetry structure of the quenched theory leads to the need to include the Φ_0.

In C we give an alternative argument for the need to keep Φ_0 in quenched, but not in PQ, theories.

IV. EFFECTIVE LAGRANGIAN

We now turn to the construction of the low energy effective Lagrangian for PQ QCD. We first recapitulate the standard approach, based on the "fake" symmetry group discussed previously. We point out the problems with this approach, and spend most of this section discussing the extent to which they can be alleviated. Our conclusion is that the standard approach is appropriate when doing perturbative calculations, although the justification for using the effective theory is considerably less rigorous than for QCD itself. Some of these points have been discussed previously in the random matrix literature, e.g., in Ref. [11], although in the context of effective theories including Φ_0. Our aims here are to clarify this work, and to generalize it to the case at hand in which Φ_0 is absent. Parts of our discussion are based on an analysis of the quenched effective Lagrangian given in Ref. [17].

A. The standard approach

The fields in the effective theory can be limited to those describing the pseudo-Goldstone hadrons. These, as we have seen, are in one-to-one correspondence with the generators of

$$[SU(N_V + N|N_V)_L \otimes SU(N_V + N|N_V)_R]/SU(N_V + N|N_V)_V. \tag{28}$$

In the standard approach [10] the pseudo Goldstone fields lie in this coset space, with the parametrization

$$U(x) = \exp\left(\frac{2i\Phi(x)}{f}\right), \quad \Phi(x) = \begin{pmatrix} \phi(x) & \eta_1(x) \\ \eta_2(x) & \tilde{\phi}(x) \end{pmatrix},$$

$$\phi^\dagger = \phi, \quad \tilde{\phi}^\dagger = \tilde{\phi}. \tag{29}$$

Here the blocks correspond to quarks and ghosts, and η_1 and η_2 are independent Grassmann matrix fields. We are free to interpret η_2 as $\eta_1^\dagger$, in which case U is unitary. The absence of Φ_0 implies the constraint $\mathrm{str}(\Phi) = \mathrm{tr}\phi - \mathrm{tr}\tilde{\phi} = 0$. The symmetries are implemented as usual:

$$U \to LUR^\dagger, \quad (L,R) \in SU(N_V + N|N_V), \tag{30}$$

with the VEV $\langle U \rangle = I$ breaking the symmetry in the required way [note that U transforms like $\tilde{\Omega}$—see Eqs. (13) and (14)]. The invariant effective Lagrangian is

$$\mathcal{L}(U) = \frac{f^2}{4} \mathrm{str}(\partial U \partial U^\dagger) - \frac{f^2}{4} \mathrm{str}(\chi U^\dagger + U\chi) + \text{higher orders},$$

$$\tag{31}$$

where χ is proportional to the quark mass matrix, $\chi = 2B_0 M$, and B_0 and f are unknown parameters. Clearly this development mirrors that for QCD step by step. [Note that Eq. (31) differs from the form of the chiral Lagrangian for PQ QCD which is usually quoted: The absence of Φ_0 means that arbitrary functions of Φ_0 which might multiply each term in the PQ chiral Lagrangian are absent.]

A problem with this effective Lagrangian becomes apparent when developing perturbation theory by expanding U about its VEV. The "str" implies that the fields $\tilde{\phi}$ have kinetic and mass terms with the wrong sign, so that $\langle U \rangle = I$ is not a minimum of the action.[6] This is dealt with in the standard treatment by simply ignoring the instability. A justification for the use of "wrong sign" propagators for some of the mesons is that it implements cancelations which correspond at the quark level to the desired cancelations between valence quark and ghost loops. Actually, once Φ_0 is excluded, the connection between pseudo-Goldstone propagators and underlying quark and ghost flows is less clear, so this qualitative justification is less convincing. Clearly a better-founded treatment is desirable.

A related concern with the standard approach is that the chiral symmetry group of the PQ QCD functional integral is not $SU(N_V + N|N_V)_L \otimes SU(N_V + N|N_V)_R$, and the unbroken vector subgroup is not $SU(N_V + N|N_V)$. As explained in Appendix A, the full group is the subgroup of $SL(N_V$

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[6]Strictly speaking, this comment applies to fields living entirely within $\tilde{\phi}$. However, the anomaly constraint implies that one neutral meson must have components from both ϕ and $\tilde{\phi}$—that corresponding to the generator T_{2N_V+N-1} in Appendix B. Since $\mathrm{str}(T_{2N_V+N-1}^2) = -1$, this mixed field also turns out to have a kinetic term with the wrong sign.

$+ N|N_V)_L \otimes SL(N_V + N|N_V)_R$, in which (using the nomenclature of Ref. [18]) the "bodies" (non-nilpotent parts) of the left- and right-handed transformations are related by

$$L = \exp(i\Phi_L), \quad R = \exp(i\Phi_R),$$

$$(\Phi_L)_{gg}|_{\text{body}}^\dagger = (\Phi_R)_{gg}|_{\text{body}}, \tag{32}$$

[with $\mathrm{str}(\Phi_{L,R}) = 0$] while (as explained at the end of Appendix A) the vector group is the subgroup of $SL(N_V + N|N_V)$ in which the body of the ghost-ghost part is unitary:

$$L = R = V = \exp(i\Phi_V), \quad (\Phi_V)_{gg}|_{\text{body}}^\dagger = (\Phi_V)_{gg}|_{\text{body}}. \tag{33}$$

The coset of these symmetries can be parametrized by transformations with $L = R^{-1}$, so that

$$L = R^{-1} = A = \exp i\Phi_A, \quad (\Phi_A)_{gg}|_{\text{body}}^\dagger = -(\Phi_A)_{gg}|_{\text{body}}. \tag{34}$$

Note that aside from the condition on the body of the ghost-ghost block, Φ_A is an arbitrary, straceless matrix. One would then expect that the correct Goldstone fields live in this coset space, i.e.

$$U'(x) = \exp\left(\frac{2i\Phi'(x)}{f}\right), \quad \Phi'(x) = \begin{pmatrix} \phi'(x) & \eta_1'(x) \\ \eta_2'(x) & i\tilde{\phi}'(x) \end{pmatrix},$$

$$\tag{35}$$

$$\tilde{\phi}'|_{\text{body}}^\dagger = \tilde{\phi}'|_{\text{body}}, \quad \mathrm{str}(\Phi') = \mathrm{tr}(\phi') - i\,\mathrm{tr}(\tilde{\phi}') = 0.$$

(Note the crucial factor of i multiplying $\tilde{\phi}'$.) ϕ' is an arbitrary matrix of complex c-number fields, constrained only by the stracelessness condition on Φ'.

It turns out that neither Eq. (29) nor Eq. (35) is correct, but before discussing this point it is useful to understand how the form of the effective Lagrangian would differ were the Goldstone fields given by Eq. (35). This field transforms like $U' \to LU'R^{-1}$, with L,R given by Eq. (32). The invariant Lagrangian is constructed from U', U'^{-1}, the mass term (a spurion which transforms like U'^{-1}), and other sources. The rules for combining these are in one-to-one correspondence with those for the usual chiral Lagrangian (with $U \leftrightarrow U'$, $U^\dagger \leftrightarrow U'^{-1}$). Thus one finds that the most general Lagrangian has the standard form, Eq. (31), except that U'^{-1} appears rather than $U^\dagger$. We stress that this holds to all orders in the chiral expansion. The fact that $\mathrm{sdet}\,U' = 1$ implies that there are no additional Φ_0-like terms. One might be concerned that the resulting Lagrangian has, in general, an imaginary part. This will turn out not to be true in the final form we consider and so we do not discuss it further here.

B. The correct Goldstone manifold

Now we return to the issue of the correct Goldstone manifold to use. Clearly it should be based on the true symmetries, and thus contained within Eq. (35). The problem is that U' in Eq. (35) has too many degrees of freedom, and we must pick an appropriate sub-manifold. This issue has been

addressed by Verbaarschot and collaborators, in the context of a theory which contains Φ_0 (see e.g. Ref. [11]). They argue, based on the mathematical results of Zirnbauer [19], that the appropriate integration domain for the effective theory is the maximal super-Riemannian manifold contained in the coset of the true symmetry group and the unbroken vector group. This results in a Goldstone field parametrized by[7]

$$U''(x) = \exp\left(\frac{2i\Phi''(x)}{f}\right), \quad \Phi''(x) = \begin{pmatrix} \phi''(x) & \eta_1''(x) \\ \eta_2''(x) & i\tilde{\phi}''(x) \end{pmatrix},$$
(36)

$$(\phi'')^{\dagger} = \phi'', \quad (\tilde{\phi}'')^{\dagger} = \tilde{\phi}''.$$

This form is then inserted in the effective Lagrangian described in the previous paragraph, i.e. Eq. (31) with $U \rightarrow U''$ and $U^{\dagger} \rightarrow U''^{-1}$. This leads to a Lagrangian whose body is real.

In the following, we discuss the reasoning leading to the form (36), and address a technical difficulty which arises when extending the argument to the theory without Φ_0. We then discuss the theoretical foundations of PQ chiral perturbation theory, and along the way give further physical motivation for the choice (36).

The important differences between the parametrizations (29), (35), and (36) are in the ghost-ghost and quark-quark blocks of the exponents.[8] We begin by focusing on the former. Here the difference between the full coset space of Eq. (35) and the manifold in Eq. (36) is only that the soul of $\tilde{\phi}'$ is not required to be Hermitian while that of $\tilde{\phi}''$ is. Thus, $\tilde{\phi}'$ appears to contain more degrees of freedom than $\tilde{\phi}''$. However, since Gaussian integrals over c-numbers are independent of the soul, as long as the integrals are convergent (see Appendix A), these extra parameters can be absorbed into $\tilde{\phi}'$. Thus the two forms (35) and (36) do not differ in this respect.

They do, however, both differ from the standard parametrization, Eq. (29), by the extra factor of i. This factor resolves the stability problem raised above. If we expand either U' or U'' around I to quadratic order, then the extra factor of i^2 cancels the minus sign from the supertrace, and the kinetic terms for $\tilde{\phi}'$ or $\tilde{\phi}''$ (which are equivalent parametrizations at this order) have the correct sign for stability. This also fixes the overall sign of the kinetic term in the Lagrangian. The same discussion holds for the mass term, as long as M is proportional to the identity. We postpone discussion of the

(most relevant) case of non-degenerate masses until later, since to address this we need first to understand the effect of the absence of Φ_0.

We now turn to the quark-quark block of the exponents. The full coset space (35) contains extra fields in this block, compared to the standard form of Eqs. (29), since ϕ' is not constrained to be Hermitian. These extra fields correspond to the generators of the non-compact part of the broken symmetry group. The choice of Ref. [11] is to keep only the usual, Hermitian part of ϕ'. A technical reason for doing so is that, if one expands about $U' = I$, the kinetic term in the action (the sign of which is now fixed) is minimized in these "Hermitian" directions, but not in the "non-compact" directions. Thus, with this choice, the propagators of both ϕ'' and $\tilde{\phi}''$ have the correct signs. For the moment we will accept this as a sufficient reason for making this choice, but return to the point below when we discuss the foundations of PQ chiral perturbation theory.

C. Constraints from the absence of Φ_0

The analysis so far has not accounted for the constraints imposed by the absence of Φ_0, i.e. by the fact that only non-anomalous symmetries should be represented by the effective Lagrangian. There is no problem when we consider the full coset space of Eq. (35). The constraint is that $\mathrm{str}(\Phi') = 0$, and this can be satisfied by expanding the diagonal or "neutral" part of Φ' using the basis for diagonal straceless generators given in Appendix B:

$$\Phi'_{neu} = \sum_{a=1}^{2N_V + N - 1} \sigma'^a T_a.$$
(37)

The important point for us is that while all but one of these generators are contained entirely within either the quark or the ghost sectors, there is one generator (T_{2N_V+N-1} in our ordering) with components in both sectors. Now consider the restricted manifold of Eq. (36). Here the constraint $\mathrm{str}(\Phi'') = \mathrm{tr}\phi'' - i\mathrm{tr}\tilde{\phi}'' = 0$ is made more stringent by the fact that ϕ'' and $\tilde{\phi}''$ are Hermitian. Thus ϕ'' and $\tilde{\phi}''$ must be separately traceless, and there can be no component of Φ''_{neu} proportional to T_{2N_V+N-1}. Thus the restrictions of the manifold remove not only Φ_0, but also another neutral generator. This is a problem because, as seen in the previous section, there are long range correlations in channels with the quantum numbers of this generator. In other words, U'' is missing one of the neutral pseudo-Goldstone bosons.

This problem can be solved by a small change in U''. As we have seen, U'' was constructed so that all bosonic fields have correct sign propagators. For the neutral fields, this requires taking components in the quark sector to be real, but those in the ghost sector to be imaginary. The generator T_{2N_V+N-1} is problematic because it straddles both sectors. However, since it satisfies $\mathrm{str}(T_a^2) = -1$, and is thus ghost-like, we propose that the corresponding field, σ''^{2N_V+N-1}, should also be taken imaginary. Explicitly, we propose replacing Φ'' in Eq. (36) with

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[7]For explicit non-perturbative calculations, the authors of Ref. [11] use a different parametrization. We use the form (36) as it is closer to the standard parametrization of Eq. (29).

[8]The anticommuting parts of the exponents have the same form in all three parametrizations. We note that the constraint $\eta_1 = \eta_2^{\dagger}$ imposed in Eqs. (29) does not change the rules for Grassmann integration, in which η_1 and η_2 are treated as matrices composed of independent Grassmann variables. There are also no issues of convergence in the Grassmann integrals.

$$\Phi'' = \Phi''_{ch} + \Phi''_{neu},$$

$$\Phi''_{ch} = \begin{pmatrix} \phi''_{ch} & \eta''_1 \\ \eta''_2 & i\tilde{\phi}''_{ch} \end{pmatrix}, \quad (\phi''_{ch})^\dagger = \phi'', \quad (\tilde{\phi}''_{ch})^\dagger = \tilde{\phi}''_{ch},$$

(38)

$$\Phi''_{neu} = \sum_{a=1}^{N_V+N-1} \sigma''^a T_a + \sum_{a=N_V+N}^{2N_V+N-1} i\sigma''^a T_a.$$

Here "ch" refers to the off-diagonal, or charged, parts of the field. In this way we include all the neutral Goldstone flavors, while maintaining the anomaly constraint, and the condition that all kinetic terms have the correct sign.

This is not quite the end of the story. The convergence of the functional integral depends also on the mass term. Given the choice of Goldstone fields just described, the Goldstone boson mass matrix can be calculated, and the functional integral converges only if its real part is positive definite. As one might expect, there is competition between the sea quark masses and the valence (and ghost) ones. It turns out (the derivation is somewhat tedious but straightforward, and we do not include the details here) that the quark masses must satisfy

$$N_V \overline{\chi_V^{-1}} (N_V \overline{\chi_V} + N \overline{\chi_S}) < (N_V + N)^2. \tag{39}$$

Here $\overline{\chi_V}$ and $\overline{\chi_S}$ are the average valence and sea quark masses, and $\overline{\chi_V^{-1}}$ the average inverse valence quark mass. Restricting lattice simulations to satisfy this constraint is undesirable and very likely unnecessary. Although the theoretical description of the simulations in terms of the PQ chiral effective theory is ill defined when relation Eq. (39) is violated, there is nothing special about this point in parameter space as far as the underlying PQ QCD is concerned. Thus, the simulations will show no special behavior when Eq. (39) is violated. In addition, chiral perturbation theory is insensitive to these global convergence considerations, and if *it* is regular at this point, and provides an adequate description of low energy PQ QCD when the quark masses are such that the inequality is satisfied, it is unlikely that the chiral expressions derived from this theory will suddenly cease to make sense just when the inequality becomes an equality.

Aside from this point, our construction has yielded an effective Lagrangian with the correct number of Goldstone fields (i.e. the same number as there are independent Ward identities), and which one can consistently expand about $\langle U'' \rangle = I$. While in principle one can work with this Lagrangian, it is more convenient for perturbative calculations to change variables as follows:

$$\tilde{\phi}''_{ch} = -i\tilde{\phi}_{ch}, \quad \sigma''^a = -i\sigma^a, \quad a = N_V+N, 2N_V+N-1,$$

(40)

$$\eta''_{1,2} = \eta_{1,2}, \quad \phi''_{ch} = \phi_{ch}, \quad \sigma''^a = \sigma^a, \quad a = 1, N_V+N-1.$$

The effect of this change is that U'' now appears to have the form of U in Eq. (29). Since the underlying integrations are unaltered, the only effect of this change of variables is to shuffle factors of i between propagators and vertices (and possibly external fields). For example, all the charged $\tilde{\phi}$ propagators now have an overall "wrong" sign, while vertex factors appear to satisfy the graded $SU(N_V+N|N_V)$ symmetry. Indeed, we can now pretend that $U \in SU(N_V+N|N_V)$, and ignore the subtleties of this section, as long as we use the prescription that wrong sign kinetic terms lead to wrong sign propagators.

D. Foundations of PQ chiral perturbation theory

As promised, we now return to the foundations of PQ chiral perturbation theory. We first revisit the issue of the extra "non-compact" generators in the quark sector. Since this sector is a simple generalization of QCD, the construction and justification of its effective low energy theory is well understood (see, e.g. Refs. [4,20]). In particular, the issue of extra generators arises also in QCD itself, though it is rarely discussed.

It is useful to recall the steps needed to construct the effective Lagrangian for QCD-like theories with N_f flavors. First, one derives the Ward identities following from the chiral symmetries. Second, given the assumed VEV, Goldstone's theorem determines that there is one light pion field for each axial current. Third, one assumes pion dominance of correlation functions, i.e. that the light fields are the only relevant degrees of freedom. One then writes down the most general local Lagrangian incorporating these degrees of freedom, which is invariant under the chiral symmetries, and asserts that this will yield the most general amplitudes consistent with the Ward identities and the principles of relativistic quantum mechanics [4]. To formalize this, one introduces sources for currents, scalar and pseudoscalar densities, etc., and defines the generating functional in the usual way

$$Z_{QCD}[f_L^\mu, f_R^\mu, S, P, \ldots] = 1 + \int \langle j_\mu^L(x) \rangle f_L^\mu(x) + \ldots.$$

(41)

The Ward identities of the theory are encapsulated in the invariance of Z under gauge-like transformations,

$$f_L^\mu \to L f_L^\mu L^{-1} - i[(\partial^\mu L)]L^{-1},$$

$$f_R^\mu \to R f_R^\mu R^{-1} - i[(\partial^\mu R)]R^{-1}, \tag{42}$$

$$S - iP \to L(x)[S - iP]R^{-1}(x),$$

$$S + iP \to R(x)[S + iP]L^{-1}(x).$$

A similar definition is used for $Z_{eff}[f_L^\mu, f_R^\mu, S, P, \ldots]$. The claim is that, by adjusting the coefficients in the effective Lagrangian, including contact terms, one can match the generating functional between QCD and the effective theory,

$$Z_{eff}[f_L^\mu, f_R^\mu, S, P, \ldots] = Z_{QCD}[f_L^\mu, f_R^\mu, S, P, \ldots], \tag{43}$$

to any desired accuracy in a momentum and quark mass expansion [20].

The issue at hand is what group the transformations L and R belong to. This depends on whether Z_{QCD} is defined using the operator formulation or with a functional integral. In the former case, the transformations of ψ and $\psi^\dagger$ are related, since $\bar{\psi} = \psi^\dagger \gamma_0$. Thus only unitary chiral transformations are symmetries [as in Eq. (7)], and $L(x)$ and $R(x)$ in (42) are elements of $SU(N_f)$. On the other hand, in the functional integral formulation, the fact that ψ and $\bar{\psi}$ are independent variables leads to a larger symmetry (see Appendix A): $L, R \in SL(N_f)$. Which of these symmetries should Z_{eff} respect? The answer is the smaller, unitary symmetry. This can be seen in two ways. First, the "extra" transformations contained in $SL(N_f)/SU(N_f)$ lead to non-Hermitian sources S and P [see Eq. (42)], and so to a non-Hermitian Hamiltonian. Thus they move us out of the space of physical theories. Second, as shown in Appendix A, the extra transformations do not lead to additional Ward identities, and thus do not lead to additional Goldstone bosons. Since the effective Lagrangian should certainly respect the symmetries of the operator formulation of the theory, and this leads to all the desired Goldstone bosons, one should not extend the effective theory to include non-compact symmetries. We conclude that the "normal" choice of pion fields in the quark block of the Goldstone matrix, Eq. (36), is correct. The only exception is for the part of ϕ'' proportional to the identity in this block (i.e. the field σ''^{2N_V+N-1}). The argument just given does not apply to this field since it is a flavor singlet in the quark block.

Finally, we address the extent to which one can derive the effective Lagrangian in the graded sector of the theory (i.e. the parts involving ghosts). The first two steps followed in the quark sector go through in this sector as well: the Ward identities of PQ QCD are the graded generalizations of those in QCD, and the symmetry breaking pattern in PQ QCD follows from that in QCD. From these results, we have established the presence of massless poles in two-point functions of broken symmetry generators. In the standard approach, the next step is to interpret each pole as being due to a physical single particle state created by the corresponding operator, from which follows the result that any correlation function including these operators will have poles at the same positions. This deduction is key in justifying the effective chiral Lagrangian for QCD, but its extension to PQ QCD is not obvious. Furthermore, when one includes quark masses as small perturbations in QCD, one concludes from similar arguments that this results in a small shift in the position of the poles. In PQ QCD, on the other hand, quark masses have a substantially different effect–they can lead to the appearance of a double pole at $p^2 = 0$ with a coefficient proportional to the quark masses, as will be seen explicitly in Sec. VI.

What is lacking in the PQ case is a positive-norm Hilbert space interpretation, since the theory contains ghosts. This is not to say that a derivation of the effective Lagrangian is not possible for PQ theories, but rather that a generalization of the standard methods is needed. Since quark and ghost correlation functions differ simply by signs, we speculate that the appropriate theoretical framework only differs from the standard one by requiring a vector space with indefinite metric (e.g. single anti-ghost states having negative norm), as well as bosonic ghost creation and annihilation operators. The Hamiltonian would still be physical—having real eigenvalues bounded from below—and ghost operator commutators would be causal. In this way Lorentz invariance is maintained, while unitarity is lost because of transitions between positive and negative norm states.[9] It is perhaps plausible in such a set-up that a generalization of standard "pologoy" could be derived, in turn leading to an effective Lagrangian, and that the requirement of Lorentz invariance would force this Lagrangian to be local.

V. INTEGRATING OUT THE Φ_0

The work of the previous section has shown that we can write the effective chiral Lagrangian for the PQ theory in terms of an $SU(N_V+N|N_V)$ field U, transforming as in Eq. (30). In this section we need only write the form of this Lagrangian schematically:

$$\mathcal{L}(U) = \sum_i l_i O_i(U), \qquad (44)$$

where the l_i are unknown parameters, and O_i are operators constructed from $U, U^\dagger$, their derivatives, the rescaled mass matrix χ, and sources for external operators. We note that the operators allowed by the graded chiral symmetry are identical in form to those allowed by the usual chiral symmetry in QCD. In particular, there are no additional operators.

An important property of PQ chiral perturbation theory is that correlation functions involving external sources restricted to lie within the sea-quark sector are identical to those obtained using the effective chiral Lagrangian for unquenched QCD (with $N_f = N$, and without the η'). This identity, which is trivial at the quark level, can be seen diagrammatically in chiral perturbation theory, due to cancellations between diagrams in which a valence quark is replaced with a ghost quark. A compelling general argument in support of this fact, though not a proof, is the following. Let $\mathcal{M}$ be the mass matrix for a specific valence quark and the corresponding ghost, $\mathcal{M} = \text{diag}(m_V, m_V)$. Let A be an operator which does not depend on this valence-ghost pair. We write its expectation value as $\langle A \rangle = a(\mathcal{M})$, making only the $\mathcal{M}$ dependence explicit. The flavor symmetry group includes $SU(1|1)$ transformations that mix the valence and ghost quark fields. These transformations are equivalent to a change of variables in the functional integral, in addition to a group transformation (by conjugation) of $\mathcal{M}$. Since A is unchanged by the change of variables, it follows that $a(\mathcal{M})$ can depend only on $SU(1|1)$ invariants constructed from $\mathcal{M}$. These, however, can only be supertraces of powers of the mass matrix $\text{str}(\mathcal{M}^n) = 0$, so a is independent of the valence (and ghost) quark mass. To show independence of a on the

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[9]This is indeed the structure observed in explicit calculations of scattering amplitudes in quenched chiral perturbation theory: the results are Lorentz invariant but not unitary [21].

existence of the valence-ghost fields in the theory one still needs to show that any effect from these fields introduces $\mathcal{M}$ dependence.

It follows that, with external sea-sector sources, one can restrict the internal U field to take the following block-diagonal form

$$U_{\text{QCD}} = (I_{N_V}, SU(N), I_{N_V}). \tag{45}$$

Since the terms in $\mathcal{L}(U)$ are in one-to-one correspondence with those in the QCD effective Lagrangian, and the restriction (45) does not change the form of the operators,[10] it follows that both PQ and unquenched Lagrangians share the parameters l_i. As we emphasized in [1,3], this means that the parameters l_i, which describe the chiral expansion for the unphysical PQ theory, are in fact physical. For example, at NLO, l_i are the GL coefficients which encode our current experimental knowledge (and ignorance) of QCD at low energies for the light mesons. We stress that the l_i do depend on N, i.e. the GL parameters that one obtains depend on the number of light sea quarks.

From a theoretical point of view, this completes the construction of the PQ chiral effective Lagrangian, and the demonstration that it contains only physical parameters. When doing perturbative calculations with this Lagrangian one must, however, implement the constraint that sdet $U = 1$, or, if we write $U = \exp(2i\Phi/f)$, that str$(\Phi) = 0$. A standard way of achieving this is using straceless generators. For the realistic case of $N_f = 3$ and considering only mesons, $N_V = 2$, calculations involve the generators of $SU(5|2)$, and can be quite tedious. In this section we point out that a simple alternative is to reintroduce the Φ_0 field—as a calculational device and not as a physical field—and then to integrate it out. This allows one to work in the "quark basis," rather than with the actual pseudo-Goldstone fields. Calculations in the quark basis are more transparent since one can trace quark flow through each diagram, and see the cancelations between valence quarks and ghosts very simply [14,22]. Keeping Φ_0 also allows us to reinterpret previous calculations, which have included it as a physical field, as applying to the theory without this field (a point discussed at the end of this section).

A. Functional integral approach

We reintroduce Φ_0 by enlarging U to $\Sigma \in U(N_V + N | N_V)$,

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[10]With Eq. (45), χ, U and ∂U are proportional to matrices of the general form

$$\begin{pmatrix} A & 0 & 0 \\ 0 & B & 0 \\ 0 & 0 & A \end{pmatrix}, \tag{46}$$

where the three entries correspond to valence, sea, and ghosts, and A, B stand for any $N_V \times N_V$ and $N \times N$ blocks, respectively. Any product of such matrices still has this structure, which causes each supertrace in the Lagrangian to reduce to a simple trace over the sea-sea block.

$$\Sigma(x) = U(x) \exp\left(\frac{2i\Phi_0(x)}{f\sqrt{N}} \right), \tag{47}$$

and considering a theory with Lagrangian

$$\mathcal{L}'(\Sigma) = m_0^2 \Phi_0^2 + \mathcal{L}(\Sigma) \tag{48}$$

$$= m_0^2 \Phi_0^2 + \sum_i l_i O_i(\Sigma). \tag{49}$$

In other words, we simply replace U with Σ in all the terms in $\mathcal{L}(U)$ and add a mass term for Φ_0. It is useful to make the Φ_0 dependence explicit by expanding Σ:

$$\mathcal{L}(\Sigma) = \mathcal{L}(U) + \sum_{j=1}^{\infty} R_j(U, \partial)(\Phi_0)^j, \tag{50}$$

where we allow $R_j(U, \partial)$ to contain derivatives acting on the Φ_0 field. The enlarged theory is then

$$Z = \int D\Sigma \exp\left(- \int \mathcal{L}'(\Sigma) \right) \tag{51}$$

$$= \int DU D\Phi_0 \exp\left\{ - \int \left(\mathcal{L}(U) + m_0^2 \Phi_0^2 \right. \right.$$
$$\left. \left. + \sum_j R_j(U)(\Phi_0)^j \right) \right\}. \tag{52}$$

We assume that the theory is regulated with a chirally invariant fixed cut-off, such as the lattice [23].

We now take the limit $m_0 \to \infty$, and argue that we then return to the original theory with $\Sigma \to U$, i.e. the theory that we want to do calculations with. The argument goes as follows. We expect the fluctuations in Φ_0 to be of $\mathcal{O}(1/m_0)$, and thus that all the R_i terms, which are independent of m_0, are suppressed compared to the mass term. Similarly, correlation functions calculated in this theory should become independent of R_i at $m_0 \to \infty$. Furthermore, the expectation value of any operator $O(\Sigma) = O(U) + \Sigma_j r_j(U)(\Phi_0)^j$ satisfies

$$\langle O(\Sigma) \rangle_{\mathcal{L}'} = \frac{1}{Z_{\mathcal{L}'}(m_0)} \int DU D\Phi_0 O(\Sigma) \exp\left(- \int \mathcal{L}'(\Sigma) \right) \tag{53}$$

$$\xrightarrow[m_0 \to \infty]{} \frac{1}{Z_{\mathcal{L}'}(\infty)} \int DU D\Phi_0 O(U)$$
$$\times \exp\left\{ - \int [\mathcal{L}(U) + m_0^2 \Phi_0^2] \right\} \tag{54}$$

$$= \frac{1}{Z_{\mathcal{L}}} \int DU O(U) \exp\left(- \int \mathcal{L}(U) \right) \tag{55}$$

$$= \langle O(U) \rangle_{\mathcal{L}}. \tag{56}$$

So we obtain correlation functions in the theory we want, with any Φ_0 contribution to the external operators being projected out.

It is crucial for this argument that the theory be regulated in such a way that loop momenta are limited.[11] This allows Φ_0 to be integrated out in a trivial way. Without a fixed cut-off, the $(\partial \Phi_0)^2$ term [implicitly contained in $R_2(U)\Phi_0^2$] can dominate over the m_0^2 term in loop integrals. This in turn leads to a non-decoupling of Φ_0. For example, using dimensional regularization, Φ_0 tadpole diagrams give contributions proportional to $(m_0^2/f^2)\ln(m_0/\mu_{\mathrm{DR}})$. With a fixed cut-off, by contrast, the contribution is of the form $\Lambda^4/(f^2 m_0^2)$, and vanishes when $m_0 \rightarrow \infty$.

There is a second subtlety which could invalidate the argument just presented. In physical theories heavy particles "decouple," meaning that physics at energies much lower than their mass is independent of the details of their interactions and dynamics. This idea is at the core of effective field theories in which only light particles are included as explicit dynamical degrees of freedom. In this sense, taking the mass of a particle to infinity in physical theories is well defined. For unphysical theories, however, one might be concerned that this limit does not exist. That this is a legitimate concern is shown by the fact, explained below, that the limit cannot be taken in quenched QCD. We will see, however, that this is not a problem for the PQ theory.

B. Φ_0 in the flavor-neutral propagator

To understand this point, and also to gain insight into the nature of the $m_0 \rightarrow \infty$ limit, we consider the form of the propagator of "neutral" mesons, i.e. those created by the diagonal elements of Φ. It is sufficient to consider this propagator since this is the only place that the m_0^2 term enters when one develops perturbation theory. We begin with some notation. We use $\Pi(x)$ to denote the pion field including Φ_0:

$$\Sigma = \exp\left(\frac{2i\Pi}{f}\right), \quad \Pi(x) = \Phi(x) + \Phi_0(x)\frac{I}{\sqrt{N}}. \quad (57)$$

The set of meson fields $\{\pi_{ij}\}$ that make up the quark basis is defined through

$$\Pi(x) = \sum_{i,j=1}^{2N_V+N} T_{ij}\pi^{ij}(x), \quad (T_{ij})_{kl} = \delta_{ik}\delta_{jl}, \quad (58)$$

and the flavor neutral part is therefore

$$\Pi_{\mathrm{neu}}(x) = \sum_{i=1}^{2N_V+N} T_{ii}\pi^{ii}(x). \quad (59)$$

The neutral part of Π can also be decomposed using the basis of generators of $U(N_V+N|N_V)$ given in Appendix B:

$$\Pi_{\mathrm{neu}}(x) = \sum_{a=1}^{2N_V+N} T_a\sigma^a(x), \quad (60)$$

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[11]We thank David B. Kaplan for emphasizing this point to us.

where the generators satisfy

$$\mathrm{str}(T_a T_b) = g_{ab}. \quad (61)$$

The first $2N_V+N-1$ components of σ^a are true pseudo-Goldstone fields, while the last entry is the field added by hand, Φ_0.

We consider all the quadratic terms in the action that contribute to the leading order propagator. At this point we do not specify what these terms are, only require that the Φ_0 mass term is included. For a given momentum, the inverse propagator will have the following form:

$$G_{(\sigma)}^{-1} = \begin{pmatrix} A & B \\ C & m_0^2+d \end{pmatrix}. \quad (62)$$

Here we have separated off the last row and column of the matrix, corresponding to entries involving Φ_0. Thus A [a $(2N_V+N-1)\times(2N_V+N-1)$ matrix] is the inverse propagator in the theory without Φ_0. The important point is that A, B, C and d are independent of m_0, and finite (because of the momentum cut-off). Using this, one can easily show (Appendix D) that the only requirement needed for the propagator to have a limit as $m_0 \rightarrow \infty$ is that A be non-singular. The limit is then

$$\bar{G}_{(\sigma)} = \lim_{m_0 \rightarrow \infty} G_{(\sigma)} = \begin{pmatrix} A^{-1} & 0 \\ 0 & 0 \end{pmatrix}. \quad (63)$$

This propagator has the two properties needed so that one is effectively doing the calculation using only the physical $SU(N_V+N|N_V)$ degrees of freedom: (i) its projective form removes Φ_0 from the theory—factors of Φ_0 in vertices and external fields simply do not propagate; (ii) the propagator in the physical subspace, A^{-1}, is the correct propagator for these degrees of freedom alone.[12]

Thus the only remaining question is whether A^{-1} exists. To study this we first consider only the kinetic $+m_0^2$ terms in the Lagrangian Eq. (49). A can be easily read off, using

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[12]One might be concerned that the fact that some of the fields have the wrong metric might lead to a basis dependence in the results of calculations. Indeed, the transformation between the "sigma" and "pi" bases, $\sigma^a = \Sigma_b \Lambda^a{}_b \pi^{bb}$, is not unitary, but instead is a generalized Lorentz rotation. This follows from the results

$$\mathrm{str}(\Pi_{\mathrm{neu}}^2) = \sum_{a,b} \sigma^a g_{ab}\sigma^b = \sum_{a,b} \pi^{aa}\tilde{g}_{ab}\pi^{bb}, \quad (64)$$

where g_{ab} (defined in Appendix B) plays the role of the metric tensor, and $\tilde{g}_{ab}$ has the same signature but with elements permuted. Since Lorentz-like rotations do not preserve Euclidean inner products, projections onto subspaces are not in general invariant under these rotations. This turns out, however, not to be relevant in our calculations. All that we need in order to show the basis independence of our calculations is that the propagator of the matrix field, $\langle \Pi_{\mathrm{neu}}(x)\Pi_{\mathrm{neu}}(0) \rangle$, which is the building block of perturbation theory, is the same in either basis. It is straightforward to show that for this to hold, it is sufficient for Λ to be invertible, which is clearly the case.

$$\text{str}(\partial\Pi_{neu}\partial\Pi_{neu}) \propto g_{ab}\partial\sigma^a\partial\sigma^b, \tag{65}$$

and the explicit form of g_{ab} from Appendix B:

$$\begin{aligned} \text{PQ:} \quad & A = p^2 \text{diag}(1,\ldots,1,-1,\ldots,-1,-1) \\ \text{Q:} \quad & A = p^2 \text{diag}(1,\ldots,1,-1,\ldots,-1,0). \end{aligned} \tag{66}$$

Clearly A is invertible only in the PQ case, and the limit $m_0 \to \infty$ can be taken only in that theory, but not in quenched QCD.

The usual mass term in the Lagrangian, which is of the same order in chiral perturbation theory as the kinetic term, can be treated as a vertex. This leads to a geometric series of tree diagrams, all contributing to the leading order. The propagator in these diagrams, when it exists in the $m_0 \to \infty$ limit, removes any Φ_0 contributions. This means that the conclusions derived above from Eq. (66) still hold. There is, however, a potential loophole in this argument: the infinite sum over tree level diagrams and the $m_0 \to \infty$ limit might not commute. That this is not a problem can be seen directly from previous calculations of the LO propagator in chiral perturbation theory in which the quark mass term was included before taking the $m_0 \to \infty$ limit. In the case of PQ QCD with 3 sea quarks, we have [10,3]

$$G_{AA}^{neu} \equiv \int d^4x \, e^{-ip\cdot x} \langle \pi_{AA}(x)\pi_{AA}(0) \rangle$$

$$= \frac{1}{p^2 + \chi_A}$$

$$- \frac{(p^2+\chi_1)(p^2+\chi_2)(p^2+\chi_3)(m_0^2/3)}{(p^2+\chi_A)^2(p^2+M_{\pi_0}^2)(p^2+M_\eta^2)(p^2+M_{\eta'}^2)} \tag{67}$$

$$\xrightarrow[m_0\to\infty]{} \frac{1}{p^2+\chi_A} - \frac{1}{3}\frac{(p^2+\chi_1)(p^2+\chi_2)(p^2+\chi_3)}{(p^2+\chi_A)^2(p^2+M_{\pi_0}^2)(p^2+M_\eta^2)}$$

where A is a valence quark label, χ_i normalized quark masses (with $i=1,2,3$ for sea quarks), and $M_{\pi_0}, M_\eta, M_{\eta'}$ masses of neutral mesons in the sea sector $[M_{\eta'}^2 = m_0^2 + \mathcal{O}(\chi_i/m_0^2)]$. Clearly the limit $m_0 \to \infty$ exists, so the potential problem does not arise.

The corresponding result in the quenched theory is

$$G_{AA}^{neu} = \frac{1}{p^2+\chi_A} - \frac{m_0^2/3}{(p^2+\chi_A)^2}, \tag{68}$$

which shows that the $m_0 \to \infty$ limit cannot be taken, irrespective of the quark mass. The fact that one *cannot* integrate out Φ_0 in the quenched theory is consistent with the result, discussed in Sec. III, that Φ_0 *should not* be projected out of the theory, as it contributes to long range correlations. We observe again the central role played by the structure of $\text{str}(T_aT_b)$ in the analysis.

C. Reinterpreting previous calculations

We have argued above that the Φ_0 field need not be included in PQ chiral perturbation theory because, in the massless limit, its propagator does not have a massless Goldstone pole, but instead has a pole at the η' mass (if $N=3$). Since chiral perturbation theory does not converge for $|p| \approx 1$ GeV, it will not, in general, be useful for $|p| \approx m_{\eta'}$. Thus the natural choice is leave Φ_0 out of the effective Lagrangian describing partially quenched simulations of QCD, perhaps adding it back as a mathematical device to simplify calculations, as described previously in this section.

Previous calculations in PQ chiral perturbation theory, e.g. Refs. [10,7,9,3,24], have, however, included Φ_0 as a physical field, rather than as a mathematical device. The reasons for this are partly historical (PQ chiral perturbation theory is an extension of quenched chiral perturbation theory, in which Φ_0 must be kept), and partly motivated by physics (there are regimes, e.g. large N_c or possibly $N=2$, in which Φ_0 is lighter than Λ_χ, and should be treated differently from other non-Goldstone hadrons—see also the discussion in Ref. [9]). Our purpose here is to show that these previous calculations can be used to obtain the results in the theory without Φ_0.

We recall that including Φ_0 as a physical field introduces several problems. First, chiral power counting is lost—adding a loop does not lead to an extra small factor of size m_π^2/Λ_χ^2, but rather to a factor of size m_0^2/Λ_χ^2. If this latter factor is not small, diagrams with any number of Φ_0 loops must be included. Second, because of the anomaly, one can multiply terms in the effective Lagrangian by arbitrary functions of Φ_0 consistent with parity invariance. This introduces many new and poorly known parameters. Finally, the parameters l_i are those of unquenched chiral perturbation theory including the η', which are related non-perturbatively, in a poorly known way, to those of the usual QCD chiral Lagrangian without the η'. It is possible that one can mitigate some of these problems by assuming that the additional coupling constants are small (since they are $1/N_c$ suppressed).[13] Such an analysis, however, inevitably involves assumptions which go beyond the systematic application of chiral perturbation theory.

What we note here is that if one takes the limit $m_0 \to \infty$ in the results of these calculations, one recovers the results in the theory without Φ_0 in which the parameters are those of the QCD chiral Lagrangian without the η'. The argument is a simple extension of that given in the previous section. If we expand in powers of Φ_0, the total Lagrangian is

$$\mathcal{L}''(\Sigma) = m_0^2\Phi_0^2 + \mathcal{L}(U) + \sum_{j=1}^\infty R_j'(U,\partial)(\Phi_0)^j. \tag{69}$$

This differs from Eq. (49) only in the replacement of the $R_j(U,\partial)$ terms by new functions $R_j'(U,\partial)$ which include the

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[13]Indeed, there has been significant success in applying quenched chiral perturbation theory to lattice data, despite the presence of the same problems (see, for example, Ref. [25]).

additional Φ_0 couplings. For example, a term proportional to $\alpha(\partial\Phi_0)^2$ is usually included. However, since the R'_j do not depend on m_0, the discussion of the previous section shows that they are irrelevant as $m_0\rightarrow\infty$. The remainder of the argument continues as before.

What happens to the previous calculations when $m_0\rightarrow\infty$? First, the neutral propagator goes to an m_0 independent limit—the same limit discussed in the previous section—including, in general, light single and double poles. Second, "η' loops"—those involving propagators with poles at $m'_\eta \sim m_0$—give vanishing contributions. Third, all additional Φ_0 couplings, such as α, do not contribute—as argued on general principles above. Thus the results of the calculations simplify considerably.

In fact, this simplification has been noted and used previously, though not fully justified [7–9,24]. It has been argued that, because $m_0 \sim \Lambda_\chi$, terms proportional to m_π^2/m_0^2 are higher order in chiral perturbation theory and contribute only at the two-loop level. They can thus be dropped in NLO calculations. Contributions from η' loops are not higher order (as noted above they can grow as $\ln m_0$ in dimensional regularization), but have been dropped by hand because they would not be present in QCD chiral perturbation theory calculations without the η'. Together, this amounts to integrating out Φ_0 perturbatively, whereas a non-perturbative treatment is required. Our results effectively provide such a treatment, and justify the *ad hoc* procedures adopted previously.

VI. STRUCTURE OF THE FLAVOR-SINGLET PROPAGATOR

A signature prediction of PQ chiral perturbation theory at LO and NLO concerns the peculiar features of the pole structure of correlation functions ("polology" for short). The effective theory predicts that propagators of flavor diagonal ("neutral") mesons have both single and double pole singularities. In this section we show that, with some plausible assumptions about "normal" aspects of PQ polology, the occurrence of the unphysical double poles is a consequence of the symmetry structure of the theory. It follows that the double poles really are a feature of PQ QCD, and the grounds for this important prediction of PQ chiral perturbation theory are better established and understood. We first present the argument in terms of quark fields, so that it applies directly to PQ QCD, and then point out how the argument extends to the effective theory.

A. PQ QCD

For simplicity, we discuss only the case of degenerate sea quarks.

Consider the two-point correlator of pseudoscalar quark bilinears,

$$G_{ijkl}(x)=\langle\Pi_{ij}(x)\Pi_{kl}(0)\rangle,\quad \Pi_{ij}=\mathrm{tr}(Q_i\bar{Q}_j\gamma_5). \quad (70)$$

The trace is over Dirac and color indices, and the order of Q and $\bar{Q}$ in the bilinears is chosen to simplify the transforma-

tion properties. If $i=j$ and $k=l$, we call the correlators "neutral," while if $i\neq j$ and $k\neq l$ we call them charged.[14]

We first focus on the neutral propagator in a particularly simple theory, that with a single valence quark, A, its ghost, $\widetilde{A}$, and one sea quark, S. In Appendix E we derive the constraints on G that follow from the graded vector symmetry together with Euclidian translation and rotation invariance. We find that the neutral propagator G_{jjkk} takes the following form in the $(A\bar{A},S\bar{S},\widetilde{A}\bar{\widetilde{A}})$ basis:

$$G=\begin{pmatrix} r+s & t & r \\ t & u & t \\ r & t & r-s \end{pmatrix}. \quad (71)$$

The form holds at all separations and thus also in momentum space. By following quark propagators, we can interpret the elements of G as follows. (We use the language of perturbation theory, although the results hold non-perturbatively.) The off-diagonal term $G_{AA\widetilde{A}\widetilde{A}}$ receives contributions only from disconnected diagrams, because the quark lines carrying the A flavor cannot be contracted with the $\widetilde{A}$ flavors. G_{AAAA}, on the other hand, can get contributions from both connected *and* disconnected diagrams. All the disconnected graphs contributing to either of these terms in G have exactly the same structure, except for the interchange of $\widetilde{A}$ propagators with A ones. Since these propagators are equal, and there are no relative signs from Wick contractions, it follows that r in Eq. (71) is the sum of all disconnected diagrams, and s is the sum of all connected ones.[15] Similarly, t is the sum of all disconnected diagrams but with the quark line coupled to one of the external operators replaced by a sea quark (so that $t=r$ if $m_A=m_S$). Finally, u is the complete $S\bar{S}$ propagator, including both connected and disconnected contributions. Note that the relative signs of the various contributions can be determined simply by considering Wick contractions.

Turning now to the more interesting case of $N>1$ degenerate sea quarks, it is straightforward to show that the same form of G holds for the neutral propagator in the basis in which $S\bar{S}$ is replaced by $\eta'\propto\Sigma_{j=1,N}S_j\bar{S}_j$. The quantities u, r, s, and t are of course different, with u being the η' propagator. In this theory, there are $N-1$ additional neutral bilinears, but their correlators with $A\bar{A}$, $\widetilde{A}\bar{\widetilde{A}}$ and η' vanish since the latter are invariants under any symmetry transformation that involves only sea quarks, while none of the former is. Thus G is block-diagonal and we can consistently consider only the 3×3 block Eq. (71).

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[14]In the latter case, the unbroken vector symmetries require that $i=l$ and $j=k$. This can also be seen by evaluating the correlator in terms of quark propagators.

[15]One can also show, using the graded symmetries, that s is related to correlators which are clearly charged: $s=G_{\widetilde{A}AA\widetilde{A}}$ and $s=G_{ABBA}$ if $m_A=m_B$ (see Appendix E).

For future use, we separate out from G the quantity

$$G_C \equiv \mathrm{diag}(s, u, -s). \tag{72}$$

We do this because we expect these quantities to have standard pole structure. The η' propagator u is physical, and so has only single poles, with none of them being light. As for the connected propagator s, our key assumption in this section is that it has a light single-pole. This is what is predicted by PQ chiral perturbation theory at LO and NLO [3], and also what is observed in numerical simulations of PQ theories.

In order to better understand the properties of the elements of G, it is useful to study the form of its inverse:

$$G^{-1} = \begin{pmatrix} R+S & T & -R \\ T & U & -T \\ -R & -T & R-S \end{pmatrix} \tag{73}$$

with

$$R = -\frac{ur-t^2}{us^2}; \quad S = \frac{1}{s}; \quad T = -\frac{t}{us}; \quad U = \frac{1}{u} \tag{74}$$

$$r = -\frac{UR-T^2}{US^2}; \quad s = \frac{1}{S}; \quad t = -\frac{T}{US}; \quad u = \frac{1}{U}. \tag{75}$$

We now decompose G^{-1} as

$$G^{-1} = G_C^{-1} + \Sigma, \tag{76}$$

where

$$\Sigma = \begin{pmatrix} R & T & -R \\ T & 0 & -T \\ -R & -T & R \end{pmatrix}. \tag{77}$$

The form of Eq. (76) is the same as that in perturbation theory, with G_C corresponding to the free propagator, and Σ to the one-particle irreducible self-energy. Thus we interpret Σ as the self-energy contributions arising from disconnected diagrams involving at least some valence quarks or ghosts (disconnected contributions involving sea quarks having already been included).

We can now state our second assumption: that the elements of Σ (R and T) are regular in momentum space at the position of the light pole in s. Our reasoning here is that Σ is one-particle irreducible with respect to the connected propagator, and thus does not have simple light poles. The only source for non-analyticity at the position of the light pole would be a deeply bound state of pseudo Goldstone bosons, but this should not be present because the interactions are weak.

Given our assumptions, we can now read off the pole stucture of G, by expressing it in terms of quantities with known, or assumed, behavior (simple light poles in s, around which u, R, and T are regular):[16]

$$G = \begin{pmatrix} s-Rs^2+T^2us^2 & -Tus & T^2us^2-Rs^2 \\ -Tus & u & -Tus \\ T^2us^2-Rs^2 & -Tus & -s-Rs^2+T^2us^2 \end{pmatrix}. \tag{79}$$

Thus we see that there are light double poles (the s^2 terms), but no higher order poles. A more detailed analysis shows that the residues of the double poles vanish when $m_A = m_S$.

This completes the argument for a single valence quark. What if there are two or more valence quarks? At the quark level, the addition of extra valence quarks does not change any of the elements of the block of G we consider. Thus the final form of G, Eq. (79), is unchanged, and the same double poles are present. The argument holds separately for each valence quark, and thus G_{BBBB} has double poles of the same form as G_{AAAA}, etc., although R and s depend on the mass of the valence quark. The argument can be generalized to study the structure of G_{AABB} (which has a double pole when $m_A = m_B$), but we do not give details here.

B. PQ chiral effective theory

The previous argument concerned two-point functions of quark bilinears Π_{ij}. In the derivation of the structure of G [Eq. (71)], however, the Lagrangian of PQ QCD played no role, and the only properties of Π_{ij} that were used were the transformation properties under vector symmetries. These properties are shared by the meson fields of PQ chiral perturbation theory, and therefore the propagators of these fields must also have the structure Eq. (71). Moreover, the statements about the analytic structure were based on the interpretation of the different components of G (the distinction between "connected" and "disconnected," "charged" and "neutral") which in turn used the language of Feynman diagrams and the tracing of quark lines. As discussed in Sec. V, the effective theory can be formulated with Φ_0, in which case the use of this language is still justified.

It follows that in PQ chiral perturbation theory, with Φ_0 included, if the propagators for the charged mesons have only single poles, and the self-energy function is analytic at low momentum, then there are double poles in the neutral propagators, and no higher singularities. Since the limit $m_0 \to \infty$ is well defined for these theories, and the low energy analytic structure is independent of it, we conclude that the above discussion also applies when the Φ_0 field is removed from the effective theory.

Some of the assumptions and their implications are tested by the NLO calculation described in [3]. There we found

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[16]We note that G^{-1} can be simply inverted because the usual geometric series truncates after three terms:

$$(G_C^{-1} + \Sigma)^{-1} = G_C - G_C\Sigma G_C + G_C\Sigma G_C\Sigma G_C. \tag{78}$$

$$s = \frac{Z_A}{p^2 + M_{AA}^2}, \quad u = \frac{1}{(p^2 + M_{SS}^2)/Z_S + \delta_{SS} + m_0^2}, \quad (80)$$

$$R = m_0^2 + \delta_{AA}, \quad T = m_0^2 + \delta_{AS}. \quad (81)$$

Z_A and Z_S are wave function renormalization factors and M_{AA} and M_{SS} meson masses, the expressions for which can be found in [3]. Relevant here is the fact that they are all independent of momentum and of m_0, and that M_{SS} and M_{AA} are light. $\delta_{SS}, \delta_{AA}, \delta_{AS}$ are defined through

$$\delta_{ab} = \frac{16}{f^2} L_7 \chi_a \chi_b + \frac{1}{48\pi^2 f^2} (p^2 - \chi_a - \chi_b) \frac{1}{2} (\chi_a + \chi_b)$$

$$\times \ln\left[\frac{1}{2}(\chi_a + \chi_b)\right]. \quad (82)$$

We see that the connected contribution to the propagator for the valence quark (s) has only a simple light pole, while the pole of the full sea quark η' propagator (u) is heavy (at $p^2 = -m_0^2 + \dots$). Also, the self-energy components (R, T) are clearly analytic in momentum. Finally, we collect all the terms into G, and take the limit $m_0 \rightarrow \infty$ to get

$$G = \begin{pmatrix} s + s^2\xi & -s & s^2\xi \\ -s & 0 & -s \\ s^2\xi & -s & -s + s^2\xi \end{pmatrix}, \quad (83)$$

with

$$\xi = -\delta_{AA} + 2\delta_{AS} - \delta_{SS} - \frac{p^2 + M_{SS}^2}{Z_S}. \quad (84)$$

In summary, the argument presented above serves both as a confirmation that (given the validity of the assumptions) the pole structure of two-point functions predicted by LO and NLO PQ chiral perturbation theory is indeed that of PQ QCD, and an extension of that prediction to all orders in chiral perturbation theory.

VII. CONCLUSIONS

The role of Φ_0 in quenched and PQ chiral perturbation theory has been the main focus of this paper. We have shown that in order to reproduce the low momentum behavior of two-point correlation functions of quenched QCD, Φ_0 must be kept in the theory. On the other hand, in PQ QCD it does not give rise to long range correlations, in closer analogy to the η' in QCD, and should not be included. This point is key in carrying out the program outlined in [1–3,26] of using PQ simulations together with PQ chiral perturbation theory to determine the unknown constants that govern the low energy behavior of real QCD.[17] The central fact used in this program is that the parameters of the chiral Lagrangian in QCD (with

2 or 3 light flavors) and in PQ QCD (with the corresponding number of sea quarks) are the same. In the presence of Φ_0, however, the PQ chiral Lagrangian matches the unquenched chiral Lagrangian in which the η' field is present. The latter theory does not have a low energy expansion (for the physical values $N = 2,3$ and $N_{color} = 3$), and its relation to low energy hadron phenomenology cannot be calculated perturbatively. What we have shown is that this problem does not arise because the PQ chiral effective theory can and should be formulated without Φ_0.

In seeming contradiction to what has just been stated, there are technical benefits from keeping Φ_0 in the effective theory. In this paper we have shown how Φ_0 can be included as an auxiliary field with a mass term $m_0^2 \Phi_0^2$, and its effects can be then removed by taking m_0 to infinity. This also establishes the status of previous results in PQ chiral perturbation theory in which Φ_0 was kept. By taking $m_0 \rightarrow \infty$, all effects of Φ_0 are removed from these results, irrespective of whether other Φ_0 couplings were included.

The role of Φ_0 is tied in with the more general theme of the foundation and justification of PQ chiral perturbation theory. We have addressed this issue by attempting to repeat the line of reasoning that leads to the standard chiral Lagrangian. As a first step, we have identified the full symmetries of PQ QCD. We then argued that the symmetry breaking pattern in this theory can be derived from the symmetry breaking pattern of QCD. Goldstone's theorem, with the use of the appropriately generalized Ward identities, then leads to the conclusion that two-point correlation functions of operators associated with generators of broken symmetries have low-lying poles. We discussed at some length the construction of the effective theory for the fields that have the same quantum numbers as these operators. This theory is guaranteed to recover the low energy behavior of two-point functions of the chiral currents and densities. In the absence of a Hilbert space, however, we do not know how to show that the long range behavior of *general n*-point functions can be attributed to the singularities of the two-point functions. This is a crucial implicit assumption that is made when one uses the PQ chiral effective theory.

Lacking a general argument to justify PQ chiral effective theory, we have focused instead on one of the strikingly unphysical aspects of PQ chiral perturbation theory, the existence of light double poles in propagators of flavor-neutral mesons. We have demonstrated that the existence of these double poles (and the absence of higher singularities) follows from the assumption that the propagators of charged mesons have only simple poles.[18] The proof involves only the symmetries of the theory, symmetries that are shared by the underlying microscopic theory and the low energy effective theory. We learn two things from this result. First, that this unphysical feature of the effective theory is correctly representing the properties of the underlying PQ theory. And, second, that the pole structure seen in LO and NLO chiral

[17]First results from this program have recently been presented [27].

[18]This assumption can itself be derived in the massless theory (as in Sec. III), but not in the interesting case of massive quarks with $m_V \neq m_S$.

perturbation theory will hold also at higher orders—there will only be single and double poles.

Finally, we note that an interesting consistency check of our results can be obtained by taking the valence quark masses to be much smaller than the sea quark masses, though not so small that enhanced chiral logarithms [8], proportional to $m_S \ln m_V$, invalidate chiral perturbation theory.[19] In this regime the PQ theory has a "light" sector, with correlators having poles at $M_{\text{light}}^2 \propto m_V$, and a "heavy" sector with poles at $M_{\text{heavy}}^2 \propto m_S$. We expect the relevant degrees of freedom in the light sector to be the valence quarks and ghosts alone, and thus that it should be described by an effective *quenched* $SU(N_V|N_V)$ chiral Lagrangian. In particular, this Lagrangian should contain the quenched Φ_0^Q field, despite the absence of the Φ_0 in the underlying PQ chiral Lagrangian. We also expect that additional terms, such as $\alpha(\partial \Phi_0^Q)^2$, should appear in the quenched effective Lagrangian. This issue can be investigated analytically, since both valence and sea quarks are in the chiral regime. We have checked that our expectations are indeed borne out, by matching pole positions at one-loop obtained from the underlying PQ theory and the effective quenched theory. We find, for example, that a PQ theory having N degenerate sea quarks matches with a quenched theory having $m_0^2 = 2B_0 m_S = \chi_S$ and $\alpha = 1$ (as well as small, m_S and N dependent, shifts in B_0 and f between the two theories).

ACKNOWLEDGMENTS

APPENDIX A: REAL AND FAKE SYMMETRIES

In this appendix we discuss the symmetry group of the PQ theory defined in Eq. (1), and the resulting Ward identities. We show that, although the flavor symmetry group differs from the naive expectation $SU(N_V+N|N_V)_L \otimes SU(N_V+N|N_V)_R$, the Ward identities coincide with those derived assuming this "fake" symmetry to hold. This appendix is based in part on the analogous development for the quenched theory worked out in Ref. [17].

Quark sector symmetries

Consider first only the quark part of the action, Eq. (4),

$$\int (\bar{\psi}_L \slashed{D} \psi_L + \bar{\psi}_R \slashed{D} \psi_R + \bar{\psi}_L m \psi_R + \bar{\psi}_R \bar{m} \psi_L). \quad \text{(A1)}$$

In the massless limit it is invariant under transformations of the form

$$\psi_{L,R} \to G_{L,R} \psi_{L,R}, \quad \bar{\psi}_{L,R} \to \bar{\psi}_{L,R} G_{L,R}^{-1}, \quad \text{(A2)}$$

where G_L and G_R need only be non-singular, $G_{L,R} \in GL(N_V+N)$. Requiring that the functional measure be invariant reduces the symmetry to

$$SL(N_V+N)_L \otimes SL(N_V+N)_R \otimes U(1). \quad \text{(A3)}$$

In the following we focus on the flavor symmetries, and do not show the overall $U(1)$ phase symmetry.

The group (A3) is larger than the symmetry group of the Hamiltonian, $SU(N_V+N)_L \otimes SU(N_V+N)_R$, because $\bar{\psi} \neq \psi^\dagger \gamma_0$ in the functional integral formulation. To understand the physical significance of the enlarged symmetry, we consider the resulting Ward identities. The infinitesimal transformations take the form (choosing G_L for illustration):

$$G_L = \exp(\alpha T) \simeq 1 + \alpha T \quad \text{(A4)}$$

$$\delta \psi_L = \alpha T \psi_L, \quad \delta \bar{\psi}_L = -\alpha \bar{\psi}_L T, \quad \text{(A5)}$$

where T is an arbitrary traceless, Hermitian $(N_V+N)^2$ matrix, and the small parameter, α, is complex. The usual, unitary, symmetry transformations correspond to α being pure imaginary, and thus have half as many parameters. Choosing α to be space-time dependent, we have (still in the massless theory)

$$S \to S - \int \alpha(x) \partial_\mu j_{L\mu}^{(T)}(x), \quad j_{L\mu}^{(T)} = \bar{\psi}_L \gamma_\mu T \psi_L, \quad \text{(A6)}$$

$$O(y) \to O(y) + \alpha(y) \delta_L^{(T)} O(y), \quad \text{(A7)}$$

where $\mathcal{O}$ is a local operator.[20] Such a transformation can be seen as a change of variables in the functional integral, with unit Jacobian, and therefore leads (in the example of a single operator) to

$$0 = \delta \langle O(y) \rangle$$

$$= \int \alpha(x) \partial_\mu \langle j_{L\mu}^{(T)}(x) O(y) \rangle dx + \alpha(y) \langle \delta_L^{(T)} O(y) \rangle.$$

$$\text{(A10)}$$

Note that Eq. (A10) contains α but not α^*. Thus, although it appears that two equations can be obtained for each independent matrix T (for real and imaginary α), in fact only one Ward identity results:

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[19]This is analogous to studying the chiral $SU(2)$ theory as a limit of chiral $SU(3)$. We thank Larry Yaffe for suggesting this regime to us.

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[20]It is convenient to use a somewhat inconsistent notation in which the variations of fundamental fields and generic operators are defined differently. Thus, in the case of left-handed transformations of the quark fields

$$\psi \to \psi + \delta_L \psi, \quad \text{(A8)}$$

$$O \to O + \alpha \delta_L O, \quad \text{(A9)}$$

so that, in fact, $\delta_L \mathcal{O}$ is not an infinitesimal quantity.

$$\partial_\mu \langle j_{L\mu}^{(T)}(x) O(y) \rangle = -\delta(x-y) \langle \delta_L^{(T)} O(y) \rangle. \quad \text{(A11)}$$

Thus the unitary subgroup (imaginary α) is sufficient to generate all the Ward identities implied by the full symmetry group.

When the masses are not zero, another term is added to Eq. (A10), corresponding to the variation in the action because of the mass terms. These terms, however, like the operator $\mathcal{O}$, do not involve complex conjugates of the quark fields, and therefore their variation under the transformation involves only α. As in the massless case, this implies that there is only one Ward identity [a modification of Eq. (A11)] corresponding to each generator T.

Clearly the same analysis holds for the right-handed transformations. We conclude that the unitary subgroup, $SU(N_V+N)_L \otimes SU(N_V+N)_R$, is sufficient to generate all the Ward identities implied by the full symmetry group.

Ghost sector symmetries

In the PQ QCD partition function, Eq. (1), one integrates independently over the Grassmann fields ψ and $\bar\psi$. The integral over the commuting ghost variables, however, converges only if it has a Gaussian structure:

$$\int Dx Dx^\dagger \exp(-x^\dagger A x), \quad \text{(A12)}$$

where the Hermitian part of A must be positive definite. Since $\slashed{D}$ is anti-Hermitian, this constraint applies to the mass term. Thus in the ghost part of the action,

$$\int (\bar{\bar\psi}_L \slashed{D} \tilde\psi_L + \bar{\bar\psi}_R \slashed{D} \tilde\psi_R + \bar{\bar\psi}_L \tilde m \tilde\psi_R + \bar{\bar\psi}_R \tilde m \tilde\psi_L), \quad \text{(A13)}$$

we must identify $\bar{\bar\psi}_L = \tilde\psi_R^\dagger$ and $\bar{\bar\psi}_R = \tilde\psi_L^\dagger$. The ghost part of S_F is then:

$$\int \tilde\psi_L^\dagger \slashed{D} \tilde\psi_R + \tilde\psi_R^\dagger \slashed{D} \tilde\psi_L + \tilde\psi_L^\dagger \tilde m \tilde\psi_L + \tilde\psi_R^\dagger \tilde m \tilde\psi_R. \quad \text{(A14)}$$

The symmetries of the kinetic terms alone are thus

$$\tilde\psi_L \to G \tilde\psi_L, \quad \tilde\psi_R \to (G^{-1})^\dagger \tilde\psi_R, \quad \text{(A15)}$$

where $G \in GL(N_V)$. The anomaly reduces this $GL(N_V)$ symmetry group to a product of $SL(N_V)$ and an overall phase rotation.

Ward identities are derived from infinitesimal local transformations, $G = \exp(\alpha T) \approx 1 + \alpha T$, with T a traceless, Hermitian, $N_V \times N_V$ matrix, and α complex, leading to

$$\delta\tilde\psi_L = \alpha T \tilde\psi_L, \quad \delta\tilde\psi_R = -\alpha^* T \tilde\psi_R,$$
$$\delta\tilde\psi_L^\dagger = \alpha^* \tilde\psi_L^\dagger T, \quad \delta\tilde\psi_R^\dagger = -\alpha \tilde\psi_R^\dagger T. \quad \text{(A16)}$$

Local operators, $\mathcal{O}(\tilde\psi_L, \tilde\psi_L^\dagger, \tilde\psi_R, \tilde\psi_R^\dagger)$, transform like

$$\delta O(y) = \underbrace{\left(\frac{\partial O}{\partial \tilde\psi_L} T \tilde\psi_L - \tilde\psi_R^\dagger T \frac{\partial O}{\partial \tilde\psi_R^\dagger} \right)}_{\equiv \delta_L O} \alpha(y) - \underbrace{\left(\frac{\partial O}{\partial \tilde\psi_R} T \tilde\psi_R - \tilde\psi_L^\dagger T \frac{\partial O}{\partial \tilde\psi_L^\dagger} \right)}_{\equiv \delta_R O} \alpha^*(y). \quad \text{(A17)}$$

One obtains (for the case of the expectation value of a single operator)

$$\int_x \alpha(x) \langle \partial j_L^{(T)}(x) O(y) \rangle - \alpha(x)^* \langle \partial j_R^{(T)}(x) O(y) \rangle$$

$$= -\alpha(y) \langle \delta_L O(y) \rangle + \alpha(y)^* \langle \delta_R O(y) \rangle, \quad \text{(A18)}$$

with

$$j_{L,R\mu}^{(T)} \equiv \tilde\psi_{R,L}^\dagger \gamma_\mu T \tilde\psi_{L,R}. \quad \text{(A19)}$$

By taking α real and imaginary the full set of Ward identities are seen to be equivalent to the equations

$$\langle \partial j_{L,R}^{(T)}(x) O(y) \rangle = -\delta(x-y) \langle \delta_{L,R} O(y) \rangle. \quad \text{(A20)}$$

The generalization to $\tilde m \neq 0$ is straightforward.

The resulting identities are exactly those that one would obtain were one to pretend that $\tilde\psi$ and $\bar{\bar\psi}$ were independent, and that the symmetry group was $SU(N_V)_L \otimes SU(N_V)_R$. We note, however, that, unlike the situation in the quark sector, the true symmetry group $SL(N_V)$ does not contain the "fake" symmetry group $SU(N_V)_L \otimes SU(N_V)_R$. While they do share a common vector $SU(N_V)$ subgroup, and have the same number of generators, the axial transformations (left and right handed fields rotating oppositely) differ. We also note that the use of complex α is crucial for obtaining all the independent Ward identities.

Graded symmetries

To complete the symmetries we need to consider graded transformations which rotate Grassmann and ghost fields into each other. Once we do this, we are necessarily considering the ghost fields to be commuting elements of a Grassmann algebra, with (in the notation of Ref. [18]) both a "body" or "base"—the usual complex scalar field—and a "soul"—composed of products of an even number of Grassmann fields, and thus nilpotent. The following question thus arises: What constraint does the requirement of a convergent functional integral impose on $\bar{\bar\psi}$ and $\tilde\psi$? We argue at the end of this appendix that the answer is

$$\bar{\tilde{\psi}}_L|_{\text{body}} = \tilde{\psi}_R^\dagger|_{\text{body}}, \quad \bar{\tilde{\psi}}_R|_{\text{body}} = \tilde{\psi}_L^\dagger|_{\text{body}}, \quad \text{(A21)}$$

i.e. the relations discussed above hold for the bodies of these quantities, but not for the souls. In this subsection we discuss the consequences of this constraint on the symmetries.

To do this, we return to the notation

$$Q_{L,R}^T = (\psi_{L,R}^T, \tilde{\psi}_{L,R}^T), \quad \bar{Q}_{L,R} = (\bar{\psi}_{L,R}, \bar{\tilde{\psi}}_{L,R}). \quad \text{(A22)}$$

The most general anomaly-free flavor transformation which leaves the kinetic term

$$\int \bar{Q}_L \slashed{D} Q_L + \bar{Q}_R \slashed{D} Q_R, \quad \text{(A23)}$$

invariant is

$$\begin{aligned} Q_L \to L Q_L \quad & Q_R \to R Q_R \\ \bar{Q}_L \to \bar{Q}_L L^{-1} \quad & \bar{Q}_R \to \bar{Q}_R R^{-1}. \end{aligned} \quad \text{(A24)}$$

Here L and R are independent $SL(N_V + N|N_V)$ matrices, except that they must maintain the constraint (A21). If we write

$$L = \begin{pmatrix} L_{qq} & L_{qg} \\ L_{gq} & L_{gg} \end{pmatrix}, \quad \text{(A25)}$$

(and similarly for L^{-1}, R and R^{-1}) to denote the quark-quark block, quark-ghost block, etc., of the different matrices, then the constraint is

$$L_{gg}|_{\text{body}} = (R_{gg}^{-1})|_{\text{body}}^\dagger. \quad \text{(A26)}$$

In deriving this, we have used

$$(L^{-1})_{gg}|_{\text{body}} = (L_{gg}|_{\text{body}})^{-1} = L_{gg}^{-1}|_{\text{body}} \quad \text{(A27)}$$

and related results, which follow from the fact that only the product of "bodies" contribute to the body of a product. The matrices L and R satisfying the constraint Eq. (A26) form a subgroup of $SL(N_V + N|N_V)_L \otimes SL(N_V + N|N_V)_R$. The exponential parametrization of elements of this subgroup is

$$L = \exp(i\Phi_L), \quad R = \exp(i\Phi_R),$$
$$\text{str}(\Phi_{L,R}) = 0, \quad (\Phi_L)_{gg}|_{\text{body}}^\dagger = (\Phi_R)_{gg}|_{\text{body}}. \quad \text{(A28)}$$

To derive Ward identities we consider infinitesimal transformations of the form in Eq. (A28). Transformations in the quark-quark and ghost-ghost blocks lead only to the identities described in the previous subsections. In particular, while the full symmetry group has axial transformations in the ghost-ghost block which were not considered above [in which $(\Phi_{L,R})_{gg}$ are both pure soul] these do not lead to independent Ward identities.

Additional Ward identities do arise from purely graded transformations. These are derived by considering $i\Phi_{L,R} = \alpha_{L,R} T$, with T Hermitian matrices contained entirely in the quark-ghost and ghost-quark blocks, and $\alpha_{L,R}$ anticommuting parameters. Note that there are no constraints on $\alpha_{L,R}$ from Eq. (A28), and so the derivation of Ward identities

follows the same steps as in the quark sector, except that one must keep track of the anticommuting nature of α. The result is a single independent identity of the form of Eq. (A11) for each "off-diagonal" generator T. As in the quark sector, the identities are the same as those that follow from the unitary subgroup in which $\Phi_{L,R}$ are constrained to be Hermitian. The extra freedom of complex parameters does not lead to additional identities.

Combining the results from all infinitesimal transformations, we see that all the Ward identities could have been obtained if one had assumed the fake symmetry group $SU(N_V + N|N_V)_L \otimes SU(N_V + N|N_V)_R$.

Vector and axial transformations and currents

The VEV of Eq. (15) (and also the mass term with $M \propto I$) breaks the chiral symmetry of Eq. (A24) down to its vector subgroup:

$$L = R \equiv V \in SL(N_V + N|N_V), \quad V_{gg}|_{\text{body}} = (V_{gg}^{-1})|_{\text{body}}^\dagger. \quad \text{(A29)}$$

The corresponding "fake" group, sufficient for deriving vector Ward identities, is the subgroup $V \in SU(N_V + N|N_V)$, for which the constraint in Eq. (A29) is automatically satisfied.

The axial transformations, the generators of which are broken by the VEV, are given by

$$L = R^{-1} \equiv A \in SL(N_V + N|N), \quad A_{gg}|_{\text{body}} = (A_{gg})|_{\text{body}}^\dagger. \quad \text{(A30)}$$

Here the fake transformations have $A \in SU(N_V + N|N)$, and are not contained in the transformations of Eq. (A30) because the constraint is not satisfied.

By combining infinitesimal left- and right-handed transformations in the appropriate way, we can derive vector and axial Ward identities. They take the same form as Eq. (A11), with $L \to V, A$, and contain

$$j_{V,A\mu}^{(T)}(x) = \bar{Q}_L \gamma_\mu T Q_L(x) \pm \bar{Q}_R \gamma_\mu T Q_R(x) \quad \text{(A31)}$$

and

$$\delta_{V,A}^{(T)} O = \delta_L^{(T)} O \pm \delta_R^{(T)} O. \quad \text{(A32)}$$

The only subtlety here is that, when deriving Ward identities for graded transformations, the factor of $\alpha(y)$ which is pulled out of Eqs. (A6)–(A10) should be accompanied by the sign which results when moving α past $\bar{Q}$. This is needed to be consistent with the definition of $j_\mu^{(T)}$, and impacts the definition of $\delta^{(T)}$.

Convergence considerations

First recall that integrals over real c-numbers lead to results of the same form as over ordinary numbers [18]

$$\int_a^b dq \, f(q) = F(b) - F(a), \quad F' = f. \quad \text{(A33)}$$

Here functions of c-numbers are defined by Taylor expansions,

$$f(q)=f(q|_{\text{body}})+\sum_{n=1}^{\infty}\frac{1}{n!}(q|_{\text{soul}})^nf^{(n)}(q|_{\text{body}}), \quad \text{(A34)}$$

where the sum actually truncates because $q|_{\text{soul}}$ is nilpotent. In our case we are interested in Gaussian integrals:

$$f(q)=\exp(-mq^2), \quad a=-\infty+a|_{\text{soul}}, \quad b=+\infty+b|_{\text{soul}}, \quad \text{(A35)}$$

with Re(m) positive. Since $f^{(n)}(\pm\infty)=0$ for all n, it follows that Eq. (A33) is actually independent of the souls of a and b. Similarly, if we change variables by a quantity which is pure soul, $q'=q+\delta q$, $\delta q|_{\text{body}}=0$, we do not have to change the limits of integration.[21] This is true for an arbitrary change in soul—in particular, it does not need to be real.

Now consider a two-dimensional Gaussian integral

$$\int_{-\infty}^{+\infty}dq_1dq_2\exp[-m(q_1^2+q_2^2)]. \quad \text{(A36)}$$

As we have just seen, the bodies of $q_{1,2}$ are real, but their souls can be arbitrary without changing the value of the integral. Thus if we change to "complex" variables

$$\widetilde{q}=q_1+iq_2, \quad \bar{\widetilde{q}}=q_1-iq_2, \quad d\widetilde{q}d\bar{\widetilde{q}}\equiv dq_1dq_2, \quad \text{(A37)}$$

then the integral takes on the usual complex Gaussian form

$$\int d\widetilde{q}d\bar{\widetilde{q}}\exp(-m\bar{\widetilde{q}}\widetilde{q}), \quad \text{(A38)}$$

except that $\bar{\widetilde{q}}=\widetilde{q}^*$ holds only for the bodies, and not for the souls (since the souls of $q_{1,2}$ are not real). The integral itself has the value given by Eq. (A36), i.e. π/m. Note that m can also have an arbitrary soul—what matters for convergence is that the real part of its body is positive.

The generalization to many complex variables is straightforward. Let $\widetilde{q}$ and $\bar{\widetilde{q}}$ now represent a vector and transposed vector, respectively. Then the integral

$$\int d\widetilde{q}d\bar{\widetilde{q}}\exp(-\bar{\widetilde{q}}M\widetilde{q}) \quad \text{(A39)}$$

is convergent if M (taken to have no soul for now) is Hermitian and positive, and if $\bar{\widetilde{q}}=\widetilde{q}^\dagger$ holds for the bodies. To see this we diagonalize M: $M=U^\dagger DU$, with D being diagonal and positive, and U unitary. Thus if we use the variables $\widetilde{q}'=U\widetilde{q}$ and $\bar{\widetilde{q}}'=\bar{\widetilde{q}}U^\dagger$ (which leaves the measure unchanged), then the integral factorizes into a product of integrals of the form of Eq. (A38), each of which is convergent

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[21]Note that this is not true for general integrals: one must take care when making changes of variables involving nilpotent parts, since they can lead to so-called anomalies [11,19].

as long as $\bar{\widetilde{q}}'|_{\text{body}}=\widetilde{q}'|_{\text{body}}^\dagger$. This relation is maintained by the unitary transformation back to the unprimed fields. The argument goes through if M has an arbitrary soul, since the integrand can be expanded in powers of this soul, and each term is convergent. Note that the general symmetry transformation, Eq. (A24), maintains the Hermiticity of the body of M.

APPENDIX B: THE DIAGONAL GENERATORS OF $U(N_V+N|N_V)$

Here we collect some useful results concerning the generators of graded symmetry groups. These are represented by the Hermitian $(2N_V+N)^2$ matrices labeled T in the foregoing. Note that the same generators serve for both the true and fake symmetry groups. We consider here the properties of the diagonal generators.

Let λ_a be the N_V+N-1 diagonal generators of $SU(N_V+N)$, chosen to satisfy tr($\lambda_a\lambda_b$)=δ_{ab}. Similarly, let $\widetilde{\lambda}_a$ be the N_V-1 diagonal generators of $SU(N_V)$, normalized in the same fashion. We define T_a, $a=1,\ldots,N+2N_V-2$ to be the set of matrices:

$$\begin{matrix} N_V+N \text{ quark indices} \{ \\ N_V \text{ ghost indices} \{ \end{matrix} \quad \left(\begin{array}{c|c}\lambda_a & 0 \\ \hline 0 & 0\end{array}\right), \quad \left(\begin{array}{c|c}0 & 0 \\ \hline 0 & \widetilde{\lambda}_a\end{array}\right), \quad \text{(B1)}$$

where we use a schematic notation. They satisfy

$$\text{str}(T_a)=\left\{\begin{array}{c}\text{tr}(\lambda_a) \\ -\text{tr}(\widetilde{\lambda}_a)\end{array}\right\}=0 \quad \text{(B2)}$$

and

$$\text{str}(T_aT_b)=\left\{\begin{array}{c}\text{tr}(\lambda_a\lambda_b) \\ -\text{tr}(\widetilde{\lambda}_a\widetilde{\lambda}_b) \\ 0\end{array}\right\}=\delta_{ab}\varepsilon_a. \quad \text{(B3)}$$

Two more generators need to be defined to complete the basis for the diagonal part of $U(N_V+N|N_V)$.

Partially quenched ($N\neq0$)

We choose

$$T_{2N_V+N-1}=\frac{1}{2\sqrt{NN_V(N_V+N)}}[N\bar{I}-(2N_V+N)I] \quad \text{(B4)}$$

and

$$T_{2N_V+N}=\frac{1}{\sqrt{N}}I, \quad \text{(B5)}$$

where

$$\bar{I}\equiv(\delta_{ab}\varepsilon_a)=\left(\begin{array}{c|c}I & 0 \\ \hline 0 & -I\end{array}\right). \quad \text{(B6)}$$

The last element, T_{2N_V+N}, has non-vanishing supertrace, and generates the anomalous $U(1)$ factor of $U(N_V+N|N_V)$.

Considering now all $2N_V+N$ generators, it is straightforward to check that

$$(\mathrm{str}(T_aT_b))\equiv(g_{ab})=\mathrm{diag}(\underbrace{1,\ldots,1,}_{N_V+N-1}\underbrace{-1,\ldots,-1,}_{N_V-1}-1,1).$$

$$(B7)$$

Quenched $(N=0)$

In this case we choose

$$T_{2N_V-1}=I \qquad (B8)$$

$$T_{2N_V}=\frac{1}{2N_V}\bar{I}. \qquad (B9)$$

While the identity is straceless, $\bar{I}$ is not, and is taken as the generator of the anomalous $U(1)$ factor. Equation (B7) becomes

$$(\mathrm{str}(T_aT_b))\equiv(g_{ab})$$

$$=\begin{pmatrix} 1 & & & & & & & \\ & \ddots & & & & & & \\ & & 1 & & & & & \\ & & & -1 & & & & \\ & & & & \ddots & & & \\ & & & & & -1 & & \\ & & & & & & 0 & 1 \\ & & & & & & 1 & 0 \end{pmatrix}.$$

$$(B10)$$

APPENDIX C: ANOTHER ARGUMENT CONCERNING Φ_0

In this appendix we give an alternative argument concerning the status of Φ_0 in quenched and PQ chiral perturbation theory. We consider two-point functions of pseudoscalar densities,

$$G^{(T,T')}(x)=\langle\phi^{(T)}(x)\phi^{(T')}(0)\rangle, \qquad (C1)$$

where T,T' run over all the generators of $U(N_V+N|N_V)$ (and thus include the identity). For the diagonal generators, we use the basis given in Appendix B. We assume that all quark and ghost masses are equal, although they do not have to vanish.[22]

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[22]Note that the PQ theory differs from the unquenched theory (with N flavors) even if all masses are equal. This is because the extra fields in the PQ theory allow one to separately determine certain Wick contractions which always arise in certain linear combinations in the unquenched theory.

Consider first the PQ theory. As long as $N\geq2$, some of the generators lie entirely in the sea-quark sector. Choosing T and T' of this form, we can use chiral perturbation theory for QCD-like theories to infer that the resulting correlator has a pseudo-Goldstone boson (PGB) pole if $T=T'$, while flavor symmetry implies that it vanishes if $T\neq T'$. Thus we know that

$$G^{(T,T')}(x)=\delta_{T,T'}G_{\mathrm{PGB}}(x), \qquad T,T'\in T_{\mathrm{sea}}. \qquad (C2)$$

We note for future reference that $G_{\mathrm{PGB}}(x)$ is "connected" in the sense that the only contractions which contribute are those in which the two bilinears are connected by quark propagators.

We can extend this result to all the straceless generators using the graded vector symmetry (which, as argued in the text, is not spontaneously broken), with the result

$$G^{(T,T')}(x)=\mathrm{str}(TT')G_{\mathrm{PGB}}(x) \qquad \mathrm{str}(T)=\mathrm{str}(T')=0. \qquad (C3)$$

This can be shown either directly using the symmetry, along the lines of Appendix E, or by a direct comparison of the contributing contractions. In the latter case, the overall factor $\mathrm{str}(TT')$, which can be of either sign (see Appendix B), accounts for the signs arising from fermionic Wick contractions. The result (C3) shows that there are PGB poles in the correlation functions for each of the generators of $SU(N_V+N|N_V)$. This agrees with the result obtained in Sec. III B and implies that the corresponding fields should be included in the effective Lagrangian.

Now consider the correlation functions involving the interpolating field corresponding to Φ_0, which are obtained by setting T and/or T' to the identity. Flavor symmetry implies that if $T=I$ and $\mathrm{str}(T')=0$, or vica-versa, then the correlator vanishes. If $T=T'=I$, then, by inspecting contractions, one can show that the correlator is proportional to that for the η' [10]:

$$G^{(I,I)}(x)=\langle\Phi_0(x)\Phi_0(0)\rangle\propto\langle\eta'(x)\eta'(0)\rangle \qquad (C4)$$

where the η' is the flavor singlet meson *in the sea sector*. Valence quark and ghost contributions completely cancel. Now, due to the axial anomaly, we know that the η' correlator does not have a light pole. Thus none of the two-point functions involving Φ_0 have PGB poles. Conversely, to describe the long distance parts of the two-point functions in the PQ theory we do not need to consider correlators involving Φ_0.

We now contrast this analysis with that for the quenched theory. By examining contractions, or using the graded flavor symmetries, one can show that

$$G_Q^{(T,T')}(x)=\mathrm{str}(TT')G_{\mathrm{conn}}(x)+\mathrm{str}(T)\mathrm{str}(T')G_{\mathrm{disc}}(x),$$

$$(C5)$$

where "conn" and "disc" refer to connected and disconnected contractions, and T and T' run over the generators of $U(N_V|N_V)$. Since there is no sea sector in the quenched theory, we cannot rely on experience with QCD to imply that

there are PGB poles in some channels. Instead, based on numerical data, we assume that there is such a pole in the connected correlator $G_{\text{conn}}(x)$. Then we see from Eq. (C5) that, if we use the basis explained in Appendix B, there is a PGB pole in correlators corresponding to all the generators of $SU(N_V|N_V)$ except $T=I$. This if because, for such generators, $\text{str}(T^2)\neq 0$ [so the first term in Eq. (C5) is present] but $\text{str}(T)=0$ (so the second term is absent). However, for $T=T'=I$, both $\text{str}(T)$ and $\text{str}(TT')$ vanish, and so $G_Q^{(I,I)}(x)=0$. On the other hand, if $T=I$ and $T'=\bar{I}$ (the anomalous generator), or vica-versa, then $\text{str}(TT')\neq 0$, and so

$$G_Q^{(I,\bar{I})}\propto G_{\text{conn}}(x). \tag{C6}$$

Thus this cross-correlator also has a PGB pole. Finally, if $T=T'=\bar{I}$, then

$$G_Q^{(\bar{I},\bar{I})}\propto G_{\text{disc}}(x), \tag{C7}$$

about which the present analysis says nothing, although quenched chiral perturbation theory predicts a double PGB pole.

The important conclusion is that, to include all channels which have PGB poles in them one must include both $\phi^{(\bar{I})}$ and $\phi^{(I)}\propto\Phi_0$.

APPENDIX D: G^{-1} IN THE LIMIT $m_0\rightarrow\infty$

In this section we calculate the propagator $G_{(\sigma)}$ in the large m_0 limit, where the inverse propagator is given by

$$G_{(\sigma)}^{-1}=\begin{pmatrix} A & B \\ C & m_0^2+d \end{pmatrix}, \tag{D1}$$

with A, B, C, and d independent of m_0. Note that A is a square matrix, B and C a column and row vectors, respectively, and d a number. Since d appears only in the combination m_0^2+d it can be dropped in the large m_0 limit.

We write

$$G_{(\sigma)}=\begin{pmatrix} A' & B' \\ C' & d' \end{pmatrix}. \tag{D2}$$

To learn about the m_0 dependence of the blocks of $G_{(\sigma)}$ we consider the equation

$$G_{(\sigma)}G_{(\sigma)}^{-1}=I. \tag{D3}$$

One of the equations contained in Eq. (D3) is

$$C'A+d'C=0, \tag{D4}$$

which implies $d'\sim C'$, where the tilde refers to the scaling with m_0.

Another equation in Eq. (D3) is

$$C'B+d'm_0^2=1. \tag{D5}$$

Since d' and C' scale the same, only the second term on the left hand side of Eq. (D5) is important when $m_0\rightarrow\infty$, and we conclude that

$$d',C'\sim\frac{1}{m_0^2}. \tag{D6}$$

Similarly, from

$$A'B+B'm_0^2=0 \tag{D7}$$

we get

$$B'\sim\frac{1}{m_0^2}A', \tag{D8}$$

which is then used in

$$A'A+B'C=1 \quad\underset{m_0\rightarrow\infty}{\rightarrow}\quad A'A=1. \tag{D9}$$

In the last equation we see that $G_{(\sigma)}^{-1}$ cannot be inverted when $m_0\rightarrow\infty$ unless A is a non-singular matrix.

Putting everything together, in the large m_0 limit

$$A'=A^{-1}+\mathcal{O}\left(\frac{1}{m_0^2}\right)=\mathcal{O}(1), \tag{D10}$$

$$B',C',d'=\mathcal{O}\left(\frac{1}{m_0^2}\right), \tag{D11}$$

and therefore

$$\lim_{m_0\rightarrow\infty}G_{(\sigma)}=\begin{pmatrix} A^{-1} & 0 \\ 0 & 0 \end{pmatrix}. \tag{D12}$$

APPENDIX E: THE STRUCTURE OF THE PROPAGATOR FROM GRADED SYMMETRIES

In this appendix we derive the constraints on the structure of the pion propagator that imply the form Eq. (71). The following symmetries are used:

(i) Independent phase rotations of individual flavors. These form a subgroup of the vector transformations, Eqs. (A24)–(A29), where one takes

$$V=\text{diag}(\exp\theta_A,\exp\theta_S,\exp\theta_{\tilde{A}}), \tag{E1}$$

and θ_A, θ_S and $\theta_{\tilde{A}}$ are independent. Under a phase rotation of only the flavor m,

$$G_{ijkl}\rightarrow G_{ijkl}\exp(\theta_m(\delta_{im}-\delta_{jm}+\delta_{km}-\delta_{lm})). \tag{E2}$$

(ii) $SU(1|1)$ transformations that involve only A and $\tilde{A}$. These too are vector transformations, this time with

$$V = \begin{pmatrix} a & 0 & b \\ 0 & 1 & 0 \\ c & 0 & d \end{pmatrix}, \qquad (E3)$$

where

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \in SU(1|1). \qquad (E4)$$

(iii) $G_{ijkl} = (-)G_{klij}$. This symmetry follows from

$$\langle \Pi_{ij}(x)\Pi_{kl}(0) \rangle = \langle \Pi_{ij}(-x)\Pi_{kl}(0) \rangle$$
$$= \langle \Pi_{ij}(0)\Pi_{kl}(x) \rangle$$
$$= (-)\langle \Pi_{kl}(x)\Pi_{ij}(0) \rangle, \qquad (E5)$$

where the first equation is obtained by rotation, the second by translation, and the $(-)$ sign in the third is only needed when both Π_{ij} and Π_{kl} are fermionic fields.

The invariance of G under transformations of the form Eq. (E2) implies that the indices must be paired up (quark lines must be followed, corresponding to legal contraction of quark fields). The non-vanishing elements of G therefore take the form G_{iijj} or G_{ijji}. The implications of the $SU(1|1)$ symmetries are slightly less straightforward. We first form the following 2-indexed objects out of the elements of G:

$$\sum_{j=A,\tilde{A}} G_{ijjk}(x) = \langle [\Pi(x)\Pi(0)]_{ik} \rangle$$

$$\sum_{j=A,\tilde{A}} \varepsilon_j G_{jjik}(x) = \langle \text{str}(\Pi(x))\Pi_{ik}(0) \rangle$$

$$\qquad\qquad (E6)$$

$$G_{SSik}(x) = \langle \Pi_{SS}(x)\Pi_{ik}(0) \rangle$$

$$G_{iSSk}(x) = \langle \Pi_{iS}(x)\Pi_{Sk}(0) \rangle.$$

The matrix notation (Π with no indices, matrix multiplication, and the strace symbol) refers to 2×2 matrices in the $A - \tilde{A}$ subspace. In a consistent manner, $i,k \in \{A,\tilde{A}\}$. All of the combinations above transform similarly under $SU(1|1)$ transformations:

$$O_{ik} \to \sum_{m,n=A,\tilde{A}} U_{im}O_{mn}U^{\dagger}_{nk}, \qquad (E7)$$

or, using the 2×2 notation again,

$$O \to UOU^{\dagger}. \qquad (E8)$$

Since $SU(1|1)$ is a symmetry, each of the combinations are invariant under these transformations. Direct examination shows that this implies that each O must be proportional to the identity. From this argument we obtain the following set of equations:

$$\sum_{j=A,\tilde{A}} G_{ijjk} = r\delta_{ik} \Rightarrow \begin{cases} G_{AAAA} + G_{A\tilde{A}\tilde{A}A} = r \\ G_{\tilde{A}AA\tilde{A}} + G_{\tilde{A}\tilde{A}\tilde{A}\tilde{A}} = r \end{cases} \qquad (E9)$$

$$\sum_{j=A,\tilde{A}} \varepsilon_j G_{jjik} = s\delta_{ik} \Rightarrow \begin{cases} G_{AAAA} - G_{\tilde{A}\tilde{A}AA} = s \\ G_{AA\tilde{A}\tilde{A}} - G_{\tilde{A}\tilde{A}\tilde{A}\tilde{A}} = s \end{cases} \qquad (E10)$$

$$G_{SSik} = t\delta_{ik} \Rightarrow G_{SSAA} = G_{SS\tilde{A}\tilde{A}} = t \qquad (E11)$$

$$G_{iSSk} = v\delta_{ik} \Rightarrow G_{ASSA} = G_{\tilde{A}SS\tilde{A}} = v. \qquad (E12)$$

Finally, with the use of Eq. (E5), these equations can be solved to yield:

$$G_{AAAA} = r + s \qquad (E13)$$

$$G_{\tilde{A}\tilde{A}\tilde{A}\tilde{A}} = r - s \qquad (E14)$$

$$G_{AA\tilde{A}\tilde{A}} = G_{\tilde{A}\tilde{A}AA} = r \qquad (E15)$$

$$G_{\tilde{A}AA\tilde{A}} = -G_{A\tilde{A}\tilde{A}A} = s \qquad (E16)$$

$$G_{SSAA} = G_{AASS} = G_{SS\tilde{A}\tilde{A}} = G_{\tilde{A}\tilde{A}SS} = t \qquad (E17)$$

$$G_{ASSA} = G_{SAAS} = G_{\tilde{A}SS\tilde{A}} = -G_{S\tilde{A}\tilde{A}S} = v. \qquad (E18)$$

The last independent element of G is G_{SSSS}. The form shown in Eq. (71) follows (what appears there is the restriction of G to the subspace of AA, SS and $\tilde{A}\tilde{A}$).

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