Flavor symmetry breaking in lattice QCD with a mixed action

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We study the phase structure of mixed-action QCD with two Wilson sea quarks and any number of chiral valence quarks (and ghosts), starting from the chiral Lagrangian. *A priori* the effective theory allows for a rich phase structure, including a phase with a condensate made of sea and valence quarks. In such a phase, mass eigenstates would become admixtures of sea and valence fields, and pure-sea correlation functions would depend on the parameters of the valence sector, in contradiction with the actual setup of mixed-action simulations. Using that the spectrum of the chiral Dirac operator has a gap for nonzero quark mass we prove that spontaneous symmetry breaking of the flavor symmetries can only occur within the sea sector. This rules out a mixed condensate and implies restrictions on the low-energy constants of the effective theory.

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I. INTRODUCTION

Dynamical lattice simulations with fermions that preserve chiral symmetry [1–3] are extremely time consuming. The numerical cost typically exceeds simulations with Wilson or staggered quarks by 1 or 2 orders of magnitude [4]. For this reason so-called mixed-action simulations have been proposed, referring to a setup with either Wilson or staggered sea quarks and domain-wall or overlap valence quarks; we will refer to such valence quarks collectively as "chiral" quarks. Even though mixed-action theories are not unitary, they are widely believed to have the correct continuum limit. A key advantage is that the valence sector preserves chiral symmetry except for soft breaking by mass terms. This is particularly beneficial for the computation of weak matrix elements.

Quite a few mixed-action simulations with staggered sea quarks have already been performed [5]. All these simulations used the configurations generated by the MILC Collaboration with Asqtad-improved staggered fermions [6]. Exploratory simulations with twisted-mass Wilson fermions [7] or clover fermions [8] in the sea sector have also been reported, and more are expected in the near future.

Mixed-action theories can be studied in chiral perturbation theory (ChPT) at nonzero lattice spacing [9–11]. In particular, the dominant source for unitarity violations can be studied analytically. The scalar correlator, for example, is a sensitive probe for unitarity violations [12–14]. It has been shown that the numerical data for the scalar correlator agree quite well with the predictions of ChPT [15–17], lending support to the validity of mixed-action ChPT in describing lattice data.

In this paper we study the phase structure of mixed-action theories with two Wilson-like sea quarks and any number of chiral valence quarks (and ghosts). We consider the "Aoki" or "large cutoff effects" regime, where quark masses are of order a^2, the lattice spacing squared. The phase diagram for theories with Wilson fermions in the sea or the valence sector has been studied by various authors [18–22], and an interesting nontrivial phase structure has been found. In the two-flavor case, depending on the sign of a low-energy constant (LEC) in the chiral Lagrangian [19], there exists either a first-order phase transition with a nonvanishing minimal pion mass or an Aoki phase [23]. The latter is characterized by the spontaneous breaking of isospin and parity symmetries, with two of the three pions turning massless. We expect these scenarios to be present in the mixed-action theory as well, but *a priori* the phase structure might be more complicated.

To make the discussion more concrete, we begin with the effective chiral theory for the case of two valence quarks. We find that, indeed, the potential of the effective theory allows for a richer phase structure. In particular, depending on the sign of a certain linear combination of LECs there is a "mixed" phase, characterized by a mixed condensate built out of a sea and a valence quark.[1]

A mixed phase of the effective chiral theory immediately raises a paradox: The mixed condensate spontaneously breaks the separate sea and valence flavor symmetries to the diagonal subgroup. As a result, the mass eigenstates are admixtures of sea and valence fields. The masses themselves depend on both the sea and the valence-quark masses. This means, for example, that the two-point function of pure-sea-pion fields would become a superposition of exponentials, all of which depend on the valence-quark mass. This putative situation is clearly inconsistent with the very setup of mixed-action theories. Indeed, in any numerical simulation, by construction the

[1]As in the Aoki phase, this condensate breaks parity.

valence and ghost determinants exactly cancel out, and pure-sea physics cannot possibly depend on the presence of valence and ghost sectors.

In order to resolve this conundrum we turn to the underlying theory, mixed-action QCD. The chiral Dirac operator of the valence sector has a gap for nonzero valence mass. Following the arguments of Ref. [24], we prove that none of the flavor symmetries of the valence-ghost sector can be broken spontaneously, for any number of valence quarks. Since a mixed condensate would necessarily break the valence-ghost flavor symmetry group, this rules out a mixed condensate.

While showing that all is well in the underlying theory, this state of affairs calls into question the reliability of the effective chiral theory, since the latter appears to allow for a mixed condensate. Specializing once more to the case of two valence quarks, we derive a mass inequality in the underlying theory that constrains the mass of mixed charged pions to be not below the smaller of pure-sea and pure-valence charged pion masses.[2] In the effective theory, this mass inequality implies an inequality on a linear combination of LECs. The latter excludes the region in the phase diagram in which a mixed phase would occur, thereby preventing the effective theory from making predictions that are inconsistent with the underlying theory.

In conclusion, the constrained effective theory gives a consistent description of the possible phase diagram of mixed-action QCD.

In Sec. II we introduce the effective potential for mixed-action QCD for the case of two chiral valence quarks and list its symmetries. In Sec. III we study patterns of spontaneous symmetry breaking at the level of the effective theory, focusing on the mixed condensate. Some technical details are relegated to the appendixes. The main results are derived in Sec. IV, and Sec. V offers our concluding remarks.

II. THE EFFECTIVE POTENTIAL FOR MIXED-ACTION QCD

The chiral effective Lagrangian for the mixed-action theory with Wilson sea and chiral valence quarks has been constructed in Refs. [9,10].[3] It is written in terms of the nonlinear field

$$\Sigma = \begin{pmatrix} \exp\left(\frac{2i}{f}\phi\right) & \bar{\omega} \\ \omega & \exp\left(\frac{2}{f}\hat{\phi}\right) \end{pmatrix}. \tag{2.1}$$

Specializing to the case of two sea and two valence quarks, ϕ is a four-by-four Hermitian matrix and $\hat{\phi}$ a two-by-two Hermitian matrix, while $\bar{\omega}$ and ω are four-by-two and two-by-four matrices, respectively, with Grassmann-valued entries.[4] We will label the rows and columns of Σ as u_s, d_s, u_v, d_v, $\tilde{u}_v$, and $\tilde{d}_v$, where u stands for up, d stands for down, and s and v stand for sea and valence, respectively, while the tilde indicates ghost quarks.

To the order we are working here the potential is [10]

$$\begin{aligned} V = &-\frac{f^2}{8}\,\mathrm{str}(\hat{m}\Sigma^{-1} + \Sigma\hat{m}) - \frac{f^2}{8}\hat{a}\,\mathrm{str}(P_S\Sigma^{-1} + \Sigma P_S) \\ &- \hat{a}^2 W_M\,\mathrm{str}(T_3\Sigma T_3\Sigma^{-1}) \\ &- \hat{a}^2 W_8'\,\mathrm{str}(P_S\Sigma^{-1}P_S\Sigma^{-1} + \Sigma P_S\Sigma P_S) \\ &- \hat{a}^2 W_6'(\mathrm{str}(P_S\Sigma^{-1} + \Sigma P_S))^2 \\ &- \hat{a}^2 W_7'(\mathrm{str}(P_S\Sigma^{-1} - \Sigma P_S))^2, \end{aligned} \tag{2.2}$$

where str denotes the supertrace. Note that we need Σ^{-1} instead of $\Sigma^\dagger$, because the ghost part of this nonlinear field is not unitary. Furthermore, we have that $\mathrm{sdet}(\Sigma) = 1$, with sdet the superdeterminant. The parameters $\hat{m}$ and $\hat{a}$ are proportional to the quark mass matrix and the lattice spacing, respectively:

$$\hat{m} = 2B_0 M, \qquad \hat{a} = 2W_0 a, \tag{2.3}$$

where M is the real diagonal mass matrix. The parameters f and B_0 are the familiar LECs of continuum ChPT, while W_0, W_M, and W_i' are additional LECs associated with a nonvanishing lattice spacing. P_S is the projector on the sea-quark sector, with $P_S = (1 + T_3)/2$. Explicitly,

$$M = \begin{pmatrix} m_s\mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & m_v\mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & m_g\mathbf{1} \end{pmatrix}, \qquad P_S = \begin{pmatrix} \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix},$$

$$T_3 = \begin{pmatrix} \mathbf{1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{1} \end{pmatrix}, \tag{2.4}$$

where $\mathbf{0}$ is the two-by-two null matrix and $\mathbf{1}$ is the two-by-two unit matrix. m_s is the sea-quark mass, m_v is the valence-quark mass, and $m_g = |m_v|$ is the ghost-quark mass, which we always choose equal in magnitude to the valence-quark mass.[5] Since the valence determinant does not depend on the sign of m_v, the ghost determinant cancels the valence determinant exactly for this choice. We assume isospin symmetry in both the sea and the valence sector.

In the following, we will absorb the contribution of order a in the potential into the definition of the sea-quark mass, which amounts to shifting $m_s \to m_s + aW_0/B_0$. This is not

[2] For a review of mass inequalities in standard QCD, see Ref. [25].

[3] For an introduction, see, for example, Ref. [26].

[4] The fact that the two-by-two matrix $\exp(2\hat{\phi}/f)$ is not unitary but Hermitian follows from a detailed study of the symmetries in the ghost sector [22,27,28].

[5] Note that m_g has to be taken positive in order for the QCD path integral in the ghost sector to be convergent. Consistently, the sign of the ghost-quark mass *cannot* be changed by a chiral symmetry transformation [22].

only convenient but also justified, since the order-a shift contributes only to the additive mass renormalization of the sea-quark mass.

In order to simplify the notation we rescale the potential by $V \to Vf^2B_0/4$, and we write

$$\begin{aligned} V = &-\mathrm{str}(M\Sigma^{-1} + \Sigma M) - c_1\,\mathrm{str}(T_3\Sigma T_3\Sigma^{-1}) \\ &- c_2\,\mathrm{str}(P_S\Sigma^{-1}P_S\Sigma^{-1} + \Sigma P_S\Sigma P_S) \\ &- c_3(\mathrm{str}(P_S\Sigma^{-1} + \Sigma P_S))^2 \\ &- c_4(\mathrm{str}(P_S\Sigma^{-1} - \Sigma P_S))^2, \end{aligned} \tag{2.5}$$

where the new coefficients c_i, $i = 1, 2, 3, 4$, are proportional to the coefficients W_M and W_i', $i = 6, 7, 8$. Note that we also absorbed the factor a^2 into the c_i, so that these LECs are now of order a^2.

In writing Eq. (2.5), we implicitly assume that all terms in V are of the same order of magnitude and equally important for the potential. In other words, we assume that we are in the Aoki regime [21] with m_v and the (shifted) mass m_s both of order a^2 in magnitude. Terms not shown in Eq. (2.5) are at least of order a^3, $ma \sim a^3$ or $m^2 \sim a^4$, with $m \sim m_v \sim m_s$.

Mixed-action QCD, and thus the effective Lagrangian and its potential, are invariant under independent flavor rotations in the sea and in the valence sector. The symmetry group G has the structure [9]

$$G = G_{\mathrm{sea}} \otimes G_{\mathrm{val}}, \quad G_{\mathrm{sea}} = \mathrm{U}(2)_V, \quad G_{\mathrm{val}} = \mathrm{U}(2|2)_V. \tag{2.6}$$

There is no symmetry connecting the sea and the valence sectors, a consequence of the different fermion formulations used in each sector in the underlying lattice theory. In the limit of vanishing lattice spacing this group enlarges to the $\mathrm{U}(4|2)_V$ symmetry of the partially quenched continuum theory [29]. For a vanishing valence-quark mass the symmetry group is larger because of the exact chiral symmetry in the valence sector. For a detailed description of the full chiral symmetry group in the valence and ghost sectors, see Refs. [22,28].

III. PATTERNS OF SPONTANEOUS SYMMETRY BREAKING

To begin our analysis, it is useful to explore the possible patterns of spontaneous symmetry breaking. We will first establish that nothing interesting happens in the ghost sector and then discuss possible symmetry-breaking patterns in the sea and valence sectors, in order to provide a context for the results that will follow in the subsequent section.

A. Ghost sector

The most general ground state has the form

$$\Sigma_{\mathrm{vac}} = \begin{pmatrix} \Sigma_q & \bar\omega \\ \omega & \Sigma_g \end{pmatrix}, \tag{3.1}$$

where Σ_q is a four-by-four matrix and Σ_g is a two-by-two matrix. A question that immediately arises is whether the Grassmann parts ω and $\bar\omega$ can acquire any nonzero vacuum expectation values. Intuitively, one would think that this cannot happen, because a Grassmann-valued scale does not exist. In Appendix A we will show that, indeed, $\omega = \bar\omega = 0$.

The constraint $\mathrm{sdet}(\Sigma_{\mathrm{vac}}) = 1$ implies that both submatrices Σ_q and Σ_g are regular and that $\det(\Sigma_q) = \det(\Sigma_g)$. To the order we are working, the block-diagonal form of the vacuum expectation value Σ_{vac} implies that the ghost and quark sectors decouple, and the potential is a sum of two terms: $V = V_q + V_g$. The two-by-two matrix Σ_g is Hermitian and positive and can be diagonalized by an isospin transformation in the ghost sector. This means that Σ_g can be written as

$$\Sigma_g = \begin{pmatrix} \rho_1 & 0 \\ 0 & \rho_2 \end{pmatrix}, \tag{3.2}$$

with $\rho_{1,2} > 0$. In terms of these two eigenvalues, the ghost-sector part of the potential then becomes equal to

$$V_g = |m_v|(\rho_1 + \rho_1^{-1} + \rho_2 + \rho_2^{-1}) + 2c_1, \tag{3.3}$$

which is minimized by $\rho_1 = \rho_2 = 1$ or, equivalently, $\Sigma_g = \mathbf{1}$.

Thus, the effective theory predicts that isospin in the ghost sector is unbroken.[6] This is in agreement with the general result we will establish in the underlying theory in Sec. IVA. As we will see next, the situation in the sea and valence sectors is more subtle.

B. Scenarios in the sea-valence sector

We begin by introducing a convenient parametrization of the most general vacuum state in the sea-valence sector. From the previous subsection we have that $\det(\Sigma_g) = 1$, and hence $\det(\Sigma_q) = 1$ as well; Σ_q is thus an element of SU(4). For future use, we subdivide Σ_q into blocks of two-by-two matrices:

$$\Sigma_q = \begin{pmatrix} \Sigma_{ss} & i\Sigma_{sv} \\ i\Sigma_{vs} & \Sigma_{vv} \end{pmatrix}. \tag{3.4}$$

Furthermore, if $\Sigma_{vv} = \rho_v\mathbf{1}$ is proportional to the unit matrix (with ρ_v a complex number), Σ_q can be written in the form

$$\Sigma_q = e^{i\phi}\begin{pmatrix} \rho_v^* D^2 & i\rho_v^\perp D \\ i\rho_v^\perp D & \rho_v\mathbf{1} \end{pmatrix}, \qquad D = \exp(i\theta\tau_3/2), \qquad \rho_v^\perp = \sqrt{1 - |\rho_v|^2}, \tag{3.5}$$

with $\phi = 0 \bmod \pi/2$, $|\rho_v| \le 1$, and in which τ_3 is the third Pauli matrix. The proof is given in Appendix B.

[6] This result generalizes to any number of flavors in the ghost sector.

Symmetries which might be spontaneously broken by the ground state are the flavor symmetry G, given in Eq. (2.6), and the discrete symmetries parity (P) and charge conjugation (C), under which the field Σ transforms according to

$$\Sigma \xrightarrow{P} \Sigma^{-1}, \qquad \Sigma \xrightarrow{C} \Sigma^{T}. \tag{3.6}$$

The vacuum state (3.5) preserves charge conjugation.[7] Parity is broken by the Aoki condensate, which corresponds to $\theta \neq 0$. The mixed condensate, which corresponds to $\rho_v^\perp \neq 0$ or, equivalently, $|\rho_v| < 1$, breaks parity too.

We now turn to a more detailed discussion of possible phases. The trivial vacuum is parametrized by $\Sigma_{ss} = \Sigma_{vv} = \mathbf{1}$ and $\Sigma_{sv} = \Sigma_{vs} = \mathbf{0}$. A first nontrivial example is provided by a vacuum expectation value of the form

$$\Sigma_q = \begin{pmatrix} e^{i\theta\tau_3} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix}, \tag{3.7}$$

with a nonvanishing isospin condensate in the sea sector [this corresponds to $\rho_v = 1$ and $\phi = 0$ in Eq. (3.5)]. This vacuum state corresponds to the Aoki phase, with spontaneous breaking of parity and flavor [23]. The nonsinglet flavor group $\mathrm{SU}(2)_{\mathrm{sea}}$ breaks down to U(1). Associated with this breaking are two massless Goldstone bosons, the charged pions $\pi^\pm_{ss}$. The possibility of the Aoki phase in the sea sector is expected, of course. It has been shown in Ref. [19] that the existence of the Aoki phase is one of two possible scenarios for unquenched lattice QCD with two flavors of Wilson fermions, which is precisely the sea sector of the mixed-action theory we study here.

A new phase, unique to the mixed-action theory, would be a phase in which Σ_{sv} and Σ_{vs} are nonzero, which corresponds to a condensate mixing sea and valence quarks. One way to explore whether such a phase might occur is to consider the meson masses obtained when the potential is expanded around the trivial vacuum, $\Sigma_q = \mathbf{1}$. Assuming m_s, $m_v \geq 0$ for the rest of this subsection and expanding the potential to quadratic order in ϕ, we find the following tree-level masses for mesons made out of two sea quarks (M_{ss}), two valence quarks (M_{vv}), and one sea and one valence quark (M_{sv}):

$$\begin{aligned} M_{ss}^2 &= B_0(2m_s + 8c_2 + 16c_3) = B_0(2m_s + 8c_2'), \\ M_{vv}^2 &= 2B_0 m_v, \\ M_{sv}^2 &= B_0(m_s + m_v + 4c_1 + 2c_2 + 8c_3) \\ &= B_0(m_s + m_v + 4c_1' + 2c_2'), \end{aligned} \tag{3.8}$$

where

$$c_1' = c_1 + c_3, \qquad c_2' = c_2 + 2c_3. \tag{3.9}$$

We note that c_4 does not contribute; it only contributes to the sea η mass through a term quadratic in η_{ss}.

[7] For other orientations of the vacuum, charge conjugation has a more complicated form that involves a flavor rotation.

First, the valence meson mass vanishes when $m_v = 0$, consistent with the fact that the valence sector has exact chiral symmetry. Second, from the expression for M_{ss}, we see that spontaneous symmetry breaking should take place in the sea sector when $c_2' < 0$ and $m_s < 4|c_2'|$, because this would drive M_{ss}^2 to a negative value. This is in agreement with the ChPT argument of Ref. [19] for the existence of an Aoki phase.

A new type of phase is suggested by the third equation of Eq. (3.8). For $2c_1' + c_2' < 0$, M_{sv}^2 becomes negative when $m_s + m_v$ is small enough. The negative curvature at the origin of field space indicates that a mixed condensate develops, alongside with mixed Goldstone bosons.

Let us explore this possibility, assuming that $c_2' > 0$ but $2c_1' + c_2' < 0$. Since $c_2' > 0$ there is no Aoki condensate in the sea sector. Furthermore, let us assume that the vacuum takes the form

$$\Sigma_q = \begin{pmatrix} \rho & i\sqrt{1-\rho^2} \\ i\sqrt{1-\rho^2} & \rho \end{pmatrix}, \tag{3.10}$$

with real ρ. [This corresponds to choosing all phases equal to zero in Eq. (3.5).] The effective potential then reduces to

$$V' \equiv \tfrac{1}{4}V - c_1 = -(m_v + m_s)\rho - (2c_1' + c_2')\rho^2. \tag{3.11}$$

If indeed $2c_1' + c_2' < 0$, we find a minimum at

$$\rho = \frac{m_v + m_s}{2|2c_1' + c_2'|}, \tag{3.12}$$

provided that the right-hand side is smaller than 1 (otherwise, the minimum is at $\rho = 1$).

Before we turn to the mass spectrum of this mixed phase, let us recall the familiar situation on the trivial vacuum. The nonlinear field is parametrized as $\Sigma = \exp((2i/f)\phi)$, where the pseudoscalar field ϕ is expanded as

$$\sqrt{2}\phi = \begin{pmatrix} \eta_{ss} + \pi^0_{ss} & \sqrt{2}\pi^+_{ss} & \eta_{vs} + \pi^0_{vs} & \sqrt{2}\pi^+_{vs} \\ \sqrt{2}\pi^-_{ss} & \eta_{ss} - \pi^0_{ss} & \sqrt{2}\pi^-_{vs} & \eta_{vs} - \pi^0_{vs} \\ \eta_{sv} + \pi^0_{sv} & \sqrt{2}\pi^+_{sv} & \eta_{vv} + \pi^0_{vv} & \sqrt{2}\pi^+_{vv} \\ \sqrt{2}\pi^-_{sv} & \eta_{sv} - \pi^0_{sv} & \sqrt{2}\pi^-_{vv} & \eta_{vv} - \pi^0_{vv} \end{pmatrix}, \tag{3.13}$$

in self-explanatory notation.[8] Disregarding the ghost sector, the flavor symmetry consists of the direct product $\mathrm{SU}(2)_{\mathrm{sea}} \otimes \mathrm{SU}(2)_{\mathrm{val}} \otimes \mathrm{U}(1)_{\text{sea-val}}$.[9] Pure-sea fields reside

[8] For example, π^+_{vs} is made of a valence antidown quark and a sea up quark, and π^-_{sv} is made of a sea antiup quark and a valence down quark. Not all fields are independent due to the constraint $\mathrm{sdet}(\Sigma) = 1$, which excludes the "supersinglet" field [29] from our effective theory.

[9] The notation $\mathrm{U}(1)_{\text{sea-val}}$ refers to a U(1) transformation with opposite phases in the sea and valence sectors. The diagonal $\mathrm{U}(1)_{\text{sea=val}}$, where these phases are equal, acts trivially on meson fields.

in the upper-left two-by-two block. They transform only under $SU(2)_{sea}$ and not under $SU(2)_{val}$.

The mixed phase is realized by an expectation value for neutral, mixed meson fields:

$$\langle \eta_{vs} \rangle = \langle \eta_{sv} \rangle = (f/\sqrt{2})\zeta, \qquad \cos\zeta = \rho. \tag{3.14}$$

This breaks the flavor symmetry spontaneously to the diagonal subgroup $SU(2)_{sea=val}$. Associated with the four broken generators are the mixed Goldstone pions

$$\begin{aligned} &\eta_{vs} - \eta_{sv}, \qquad \pi^0_{vs} - \pi^0_{sv}, \\ &\pi^+_{vs} - \pi^+_{sv}, \qquad \pi^-_{sv} - \pi^-_{vs}. \end{aligned} \tag{3.15}$$

The nonzero-mass eigenstates are admixtures of fields with different transformation properties under the separate sea and valence flavor groups. The nonvanishing masses depend on both m_s and m_v. The dependence is explicit, as well as implicit via ρ in Eq. (3.12).

Now we are facing a paradox: If, for example, we calculate the two-point function $\langle \pi^+_{ss}(0)\pi^-_{ss}(x)\rangle$, we find that it is a superposition of exponentials coming from the various nonzero-mass eigenstates of the mixed phase. These masses all depend on m_v,[10] as does the correlation function itself. But this cannot possibly be correct, because, by the very setup of mixed-action theories, the sea sector does not depend on the valence part of the action at all.

In fact, this observation is a little more subtle than it appears, because spontaneous symmetry breaking takes place in the thermodynamical limit, whereas numerical simulations are always done in finite volume.

In ChPT terminology, the analysis of the potential we have just carried out corresponds to being in the p regime for the Goldstone pions of Eq. (3.15). In order to stay in the p regime in finite volume, one would have to turn on "seeds" for the given symmetry-breaking pattern. These would take the form of mixed mass terms that couple the sea and valence quarks. Were such mass terms to be introduced at the quark level in the underlying theory, the valence and ghost determinants would no longer cancel each other. The separation into sea and valence sectors would no longer apply, and there would be nothing *a priori* wrong with finding that properties of what used to be the sea sector now depend on parameters of what used to be the valence sector.

Numerical simulations always maintain the exact cancellation of valence and ghost determinants, because rather than having the determinants of two types of quark cancel, the valence and ghost determinants are never introduced in the first place. Therefore, at this point the question arises whether we truly have a paradox. The answer is that the conflict between the effective and underlying theories is a real one. Given that no mixed mass terms ever exist in the actual mixed-action setup, we are always in the ϵ regime for the Goldstone pions of Eq. (3.15). The correct prescription in this regime is to first calculate Feynman diagrams using chiral perturbation theory for a given orientation of the condensate and then to integrate the result over all possible orientations. Let us return to our example of the two-point function $\langle \pi^+_{ss}(0)\pi^-_{ss}(x)\rangle$, but now in finite volume. On the vacuum (3.10), its leading-order (LO) value will be a superposition of exponentials, as discussed above. All other orientations of the vacuum may be obtained by the combination of $SU(2)_{val}$ and $U(1)_{val}$ rotations. These rotations leave the operators $\pi^\pm_{ss}$ invariant; hence their two-point function is unchanged when we integrate over all orientations of the mixed condensate. The finite-volume two-point function of pure-sea-pion fields would therefore depend on m_v also when we are in the ϵ regime for the Goldstone pions of Eq. (3.15). This prediction of the chiral effective theory is indeed in direct conflict with the very setup of a mixed-action numerical simulation.

IV. POSSIBLE PHASES

If the ChPT description of QCD with a mixed action is not to break down, there has to be some mechanism that excludes the mixed phase of the effective theory. This section shows that this is indeed the case: Spontaneous symmetry breaking is entirely confined to the sea sector.

In Sec. IV A we consider the valence and ghost sectors of mixed-action QCD for an arbitrary number of flavors. Following Vafa and Witten [24], we employ a bound on the spectrum of the chiral Dirac operator to prove that none of the flavor symmetries of the valence-ghost sector can break spontaneously for $m_v \neq 0$. This rules out, in particular, a mixed condensate.

In Sec. IV B we study how this information is communicated to the effective theory. We begin by deriving a mass inequality in the underlying theory, which constrains the mass of mixed charged pions to be not smaller than the minimum of the masses of pure-sea and pure-valence charged pions. Specializing (for technical reasons) to the case of two flavors of valence quarks, we infer from the mass inequality another inequality that must be satisfied by the LECs of mixed-action ChPT. The LEC inequality, in turn, excludes the range of values that produced the paradox of the previous section.

Finally, in Sec. IV C we use the results of the first two subsections to conclude that the only nontrivial phase structure occurs in the sea sector, where our analysis reduces to that of Ref. [19].

A. Absence of flavor symmetry breaking in the valence-ghost sector

In this subsection we prove that the full valence-ghost flavor symmetry group is not broken spontaneously for $m_v \neq 0$. The analysis is carried out in the underlying theory, mixed-action QCD. We first consider the valence

[10] We checked this by explicit calculation.

sector alone and then extend the result to include the ghost sector too.

In order to avoid cumbersome notation we consider a mixed-action theory with two chiral valence quarks u and d, with masses m_u and m_d.[11] At this point we assume that m_u and m_d are both nonzero but not necessarily equal. The valence-sector action is

$$S = \bar{u}Du + m_u\bar{u}(1 - \tfrac{1}{2}D)u + \bar{d}Dd + m_d\bar{d}(1 - \tfrac{1}{2}D)d, \tag{4.1}$$

where D is a lattice Dirac operator satisfying the Ginsparg-Wilson relation [30]

$$\{\gamma_5, D\} = D\gamma_5 D. \tag{4.2}$$

Following Ref. [24], we consider the isospin-breaking condensate

$$\left\langle \bar{u}\left(1-\frac{1}{2}D\right)u - \bar{d}\left(1-\frac{1}{2}D\right)d\right\rangle_A = -\frac{1}{V}\mathrm{Tr}\left(\left(1-\frac{1}{2}D\right)\left(D\left(1-\frac{1}{2}m_u\right)+m_u\right)^{-1} - [m_u \to m_d]\right). \tag{4.3}$$

The subscript A indicates a fixed gauge-field background. Assuming that D is γ_5 Hermitian, $D^\dagger = \gamma_5 D\gamma_5$, it follows from Eq. (4.2) that D is normal. Thus, D and $D^\dagger$ have a simultaneous set of eigenfunctions with eigenvalues λ and λ^*, respectively. Once again using Eq. (4.2) it follows that $\lambda + \lambda^* = \lambda^*\lambda$, so we may write

$$\lambda = 1 - e^{i\phi}. \tag{4.4}$$

Moreover, if ψ is an eigenfunction with eigenvalue λ, $\gamma_5\psi$ is an eigenfunction with eigenvalue λ^*; hence, the eigenvalues (4.4) come in pairs $\pm\phi$ (except possibly at the isolated points $\phi = 0$ or $\phi = \pi$).

Integrating over the gauge field,[12] it is now straightforward to show that the isospin-breaking condensate is equal to

$$\left\langle \bar{u}\left(1-\frac{1}{2}D\right)u - \bar{d}\left(1-\frac{1}{2}D\right)d\right\rangle = -\int_{-\pi}^{\pi} d\phi\,\rho(\phi)\left(\frac{m_u}{m_u^2 + 4\tan^2\frac{1}{2}\phi} - \frac{m_d}{m_d^2 + 4\tan^2\frac{1}{2}\phi}\right), \tag{4.5}$$

where $\rho(\phi)$ is the spectral density.[13] This clearly vanishes for $m_u - m_d \to 0$, as long as the common value $m_u = m_d$ is nonzero. The conclusion is that there is no spontaneous symmetry breaking of isospin symmetry within the valence sector.

[11]The proof generalizes trivially to any number of chiral valence quarks.

[12]The integration measure is non-negative; see below.

[13]Note that $\rho(\phi) = \rho(-\phi)$. For a similar expression for the chiral condensate with overlap fermions, see Ref. [31].

The previous analysis easily extends to the full valence-ghost sector. Since Grassmann-valued condensates cannot occur (Appendix A), this leaves us to consider a graded-symmetry-breaking condensate of the form

$$\langle \bar{q}_v(1 - \tfrac{1}{2}D)q_v + \tilde{q}^\dagger(1 - \tfrac{1}{2}D)\tilde{q}\rangle, \tag{4.6}$$

where q_v is a valence quark and $\tilde{q}$ is a ghost quark. Note the plus sign between the valence- and ghost-quark bilinears. This sign is consistent with the graded symmetries in $U(n|n)_V$ (with n the number of valence quarks), which would be broken if this condensate developed a nonvanishing expectation value.[14]

The condensate (4.6) has a spectral representation similar to Eq. (4.5), with m_u on the right-hand side replaced by the valence-quark mass m_v and m_d replaced by the ghost-quark mass m_g, which we temporarily take to be different from m_v in order to study symmetry breaking.[15] Again, in the limit $m_g \to m_v$ this condensate vanishes, for the same reasons as before, and we conclude that the full valence-ghost flavor symmetry group is not spontaneously broken.

A corollary is that no mixed condensate can ever occur. A bilinear sea-valence operator transforms in the fundamental representation of the valence-ghost symmetry group. Since this group does not break spontaneously, bilinear sea-valence operators cannot acquire nonzero expectation values.[16]

We end this subsection with a technical comment. In order to probe isospin breaking in the sea sector (where it can occur), we may have to turn on an (infinitesimal) difference Δm between the masses of the up and down sea quarks. For nonzero Δm, the two-flavor Wilson determinant is no longer positive. However, since this only happens for nonzero Δm and at a nonzero lattice spacing, the effect is of order $a\Delta m$. In this paper we work to order $m \sim a^2$ only, and so we may neglect such effects.[17]

B. Absence of mixed-phase Goldstone bosons

While in the previous subsection we showed that all is well in the underlying theory, the puzzle concerning the phase diagram of mixed-action ChPT remains to be resolved. We will begin by deriving a mass inequality relating pure-sea, pure-valence, and mixed pions in the

[14]Recall that ghost-quark fields commute with each other. For reference, the singlet condensate that does not break $U(n|n)_V$ has a minus sign between the valence and ghost terms.

[15]Recall that m_g is necessarily positive. Assuming an even number of valence quarks we may take $m_v > 0$, because, if $m_v < 0$, we have $m_v \to |m_v|$ under a nonanomalous chiral rotation of the valence quarks.

[16]The same argument excludes a valence-ghost Grassmann condensate. However, the latter was already ruled out by the general proof of Appendix A.

[17]For a discussion of why the argument of Ref. [24] does not apply to an isospin-breaking condensate in the *sea* sector, in which the quarks fields are of the Wilson type, see Ref. [19].

underlying theory. We will then infer an inequality between the LECs of mixed-action ChPT, which, as promised, excludes the region of parameters that gave rise to the paradox of Sec. III B. As in previous sections, the ChPT-level analysis is restricted to the case of two valence quarks.

We begin with the following inequality in mixed-action QCD:

$$\mathrm{tr}\,\langle (S^\dagger_{sd}(x,y) - S^\dagger_{vd}(x,y))(S_{sd}(x,y) - S_{vd}(x,y))\rangle \geq 0, \tag{4.7}$$

in which $S_{ik}(x,y)$, $i = s, v$ is the sea-, respectively, valence-quark, propagator. The second index $k = u, d$ denotes flavor, up or down.[18]

Although as it stands inequality (4.7) depends only on the d propagator, the u propagator will be encountered shortly. In the isospin-symmetric phase, the up and down propagators are equal, and Eq. (4.8) below follows from γ_5 Hermiticity of the Wilson operator.

When we get back to the effective theory, we will make use of the inequality only in the symmetric phase. Interestingly, only little extra effort is needed to extend the inequality to the phase with broken isospin (the Aoki phase), so let us make this small detour. In order to account for the latter possibility, we add a "twisted" mass term of the form $\mu\bar{q}_s i\gamma_5\tau_3 q_s$ to the (sea) Dirac operator, where $q_s = (u_s, d_s)^T$. This accomplishes two things. First, it accounts explicitly for isospin breaking. Second, it aligns isospin breaking along the third direction in isospin space, so that the relevant condensate, if it forms, would be proportional to $\bar{q}_s\gamma_5\tau_3 q_s$. We now have that

$$S^\dagger_{sd}(x,y) = \gamma_5 S_{su}(y,x)\gamma_5, \tag{4.8}$$

also when $\mu \neq 0$. Equation (4.8) holds in any finite volume and therefore also in the thermodynamical limit where μ is eventually turned off.

Using that $S^\dagger_{vd}(x,y) = \gamma_5 S_{vu}(y,x)\gamma_5$ for the chiral overlap propagator as well, inequality (4.7) can now be rewritten as

$$G_{ss}(x,y) + G_{vv}(x,y) \geq G_{sv}(x,y) + G_{vs}(x,y), \tag{4.9}$$

where

$$G_{ij}(x,y) = \langle \bar{u}_i(x) i\gamma_5 d_j(x)\bar{d}_j(y) i\gamma_5 u_i(y)\rangle. \tag{4.10}$$

There are no disconnected contributions. (This is true even if we are inside the Aoki phase, because, with our choice of the twisted-mass term, any isospin-breaking condensate must lie in the τ_3 direction.)

If inequality (4.9) holds in mixed-action QCD, it must also hold in the low-energy effective theory, in which G_{ss} corresponds to the sea-pion propagator, G_{vv} to the valence-pion propagator, and G_{vs} and G_{sv} to the mixed-pion propagators. Technically, the translation into ChPT is done by coupling the mixed-action QCD Lagrangian to pseudoscalar sources for the operators $\bar{u}_i(x)\gamma_5 d_j(x)$ and $\bar{d}_j(y)\gamma_5 u_i(y)$ [9–11,32]. While the underlying theory is nonunitary, within the effective theory the decay rates of the relevant correlation functions are thus interpreted as pion masses.

The LO result can be expressed in terms of the component fields of Eq. (3.13) as follows:

$$\langle \pi^+_{ss}(x)\pi^-_{ss}(y)\rangle + \langle \pi^+_{vv}(x)\pi^-_{vv}(y)\rangle \geq \langle \pi^+_{sv}(x)\pi^-_{vs}(y)\rangle + \langle \pi^+_{vs}(x)\pi^-_{sv}(y)\rangle. \tag{4.11}$$

Here each two-point function is a tree-level (i.e., free) propagator in the effective theory, with mass determined by the potential, Eq. (2.2). For a meson of mass M, the tree-level propagator is

$$D(x-y) = \int \frac{d^4p}{(2\pi)^4}\frac{e^{ip(x-y)}}{p^2+M^2} = \frac{M}{4\pi^2 r}K_1(Mr), \tag{4.12}$$

in which $r = |x-y|$. Substituting this into Eq. (4.11) yields the inequality

$$M_{ss}K_1(M_{ss}r) + M_{vv}K_1(M_{vv}r) \geq 2M_{sv}K_1(M_{sv}r), \tag{4.13}$$

where we used that $M_{vs} = M_{sv}$. If all masses are strictly positive, for large r we can use the asymptotic behavior of K_1,

$$K_1(z) \sim \sqrt{\frac{\pi}{2z}}e^{-z}, \qquad |z| \to \infty, \tag{4.14}$$

finding

$$M_{sv} \geq \min(M_{ss}, M_{vv}). \tag{4.15}$$

A nontrivial consequence of the mass inequality (4.15) is that the LECs appearing in Eq. (2.5), too, are subject to an inequality. To see this, we take m_s and m_v large enough that no spontaneous symmetry breaking takes place, and the curvatures at the origin of field space, which are given explicitly by Eq. (3.8), are all positive. We also choose m_v such that $M_{vv} = M_{ss}$, which implies that $m_v = m_s + 4c'_2$. We now find that the mass inequality (4.15) translates into the LECs inequality

$$2c_1 - c_2 = 2c'_1 - c'_2 \geq 0. \tag{4.16}$$

LECs are, by definition, independent of the quark masses. While we have derived the inequality by considering special values of the sea and valence masses, it must therefore hold true for arbitrary values of m_s and m_v.

We note that in our example leading up to Eq. (3.12), we assumed that $c'_2 > 0$, so that, with Eq. (4.16), $c'_1 + 2c'_2 > c'_1 - 2c'_2 \geq 0$. Therefore, $c'_1 + 2c'_2 < 0$ never occurs, and the putative vacuum solution Eq. (3.12) is never encountered.

[18]While the correlation functions under study depend on two valence flavors that we have conveniently denoted up and down, the total number of valence quarks can be any $n \geq 2$.

C. The phase diagram

We now return to the ground state [Eqs. (3.1) and (3.4)], i.e., to the minimization of the potential (2.5), but subject to the constraints we have inferred from the underlying theory.[19] In Sec. III A we found that $\Sigma_g = \mathbf{1}$. Using the result of Sec. IV A we conclude that $\Sigma_{vv} = \mathbf{1}$ as well, while using the result of both Sec. IV A and Sec. IV B it follows that $\Sigma_{sv} = \Sigma_{vs} = \mathbf{0}$. In addition, we know from Appendix A that $\omega = \bar{\omega} = 0$. Therefore, only Σ_{ss} can take on a nontrivial value, with $\det(\Sigma_{ss}) = 1$, so that $\Sigma_{ss} \in SU(2)$. Substituting the vacuum solution

$$\Sigma_{\rm vac} = \begin{pmatrix} \Sigma_{ss} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{1} \end{pmatrix} \qquad (4.17)$$

into the potential (2.5), it reduces to

$$V = -m_s \mathrm{tr}(\Sigma_{ss} + \Sigma_{ss}^\dagger) - \tfrac{1}{2} c_2' (\mathrm{tr}(\Sigma_{ss} + \Sigma_{ss}^\dagger))^2, \qquad (4.18)$$

where c_2' is defined in Eq. (3.9). This is precisely the potential which was found in Ref. [19] for QCD with two Wilson flavors and no valence sector. Depending on the sign of c_2', either isospin and parity are broken in the sea sector (if $c_2' < 0$ and $|m_s|$ is small enough), with $\pi_{ss}^{\pm}$ the corresponding Goldstone bosons, or there is a first-order phase transition (if $c_2' > 0$), with a minimum nonvanishing pion mass at nonzero lattice spacing.

In summary, adding a chiral-fermion valence sector to the dynamical Wilson-fermion theory enlarges the flavor symmetry group and, in principle, allows for many new symmetry-breaking condensates. Nevertheless, none of these condensates actually develops, and we have recovered the usual two-flavor phase diagram for the sea sector.

V. CONCLUDING REMARKS

The chiral Lagrangian for lattice QCD with a mixed action, with Wilson sea quarks and chiral valence quarks, is rather involved. We have studied this chiral Lagrangian in the case of two sea and two valence quarks in the large cutoff effects regime $m \sim a^2$. With no restrictions on the values of the order-a^2 LECs, the phase structure is rather intricate.

In particular, the effective potential appears to allow for a mixed phase with a condensate pairing valence with sea quarks. Such a mixed phase would contradict the very setup of mixed-action simulations, because pure-sea correlation functions would depend on the parameters of the valence sector.

As we have shown in this paper, the underlying theory excludes such a phase. By extending the well-known argument of Ref. [24], which relies on the existence of a gap in the spectrum of the chiral Dirac operator for nonzero mass, we have shown that none of the flavor symmetries of the valence and ghost sectors can be broken spontaneously, for any number of valence quarks. This forbids, in particular, a mixed condensate.

In addition, we have shown that the mixed-pion mass cannot be smaller than the minimum of the pure-sea and pure-valence-pion masses. This mass inequality translates into an inequality between LECs appearing in the chiral Lagrangian. The inequality, Eq. (4.16), must hold independent of the choice of action of the underlying lattice theory. In terms of the original LECs in Eq. (2.2), the bound reads

$$2W_M - W_8' \geq 0. \qquad (5.1)$$

Without this restriction on the LECs, the effective potential by itself would allow for a mixed phase. The inequality we found follows from expanding the effective potential around the trivial vacuum, i.e., Eq. (3.8), and imposing the mass inequality (4.15). It is possible that more constraints on these LECs exist that would follow from a complete study of the effective potential for arbitrary $\Sigma_{\rm vac}$, by imposing the constraints we found in the underlying theory.

Not surprisingly, we recover the well-known conclusion of Ref. [19] about the possible phase structure in the sea sector. If $c_2' > 0$, there is a first-order transition when m_s changes sign, and the pion mass is always larger than zero; if $c_2' < 0$, a second-order transition occurs for small enough m_s, in which isospin and parity are spontaneously broken [23]. This raises the question whether an inequality might also be derived for c_2' by considering the charged and neutral pion masses in the sea sector. The reason that this is not possible, however, is that the neutral pion propagator in QCD with broken isospin contains "disconnected" diagrams, so that the arguments of Sec. IV B do not apply. Note that in Sec. IV B we only considered propagators for charged pions, making sure that no disconnected contributions appear.[20]

Finally, we expect that our conclusions generalize to other mixed actions with a chiral valence sector. For instance, if the sea quarks are staggered, they might exhibit a nontrivial phase structure [33]. In a mixed-action theory with a staggered sea sector, this nontrivial phase structure would remain confined to the sea sector, just as in the case we considered in this paper.

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[19] In this paper we analyze the potential for the case of two valence quarks, but since the proof of Sec. IV A is valid for an arbitrary number of valence quarks, we expect that the analysis of the potential can be generalized accordingly.

[20] Here disconnected diagrams are diagrams with disconnected quark loops; they are still connected if also gluon lines are taken into consideration.

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APPENDIX A: ABSENCE OF GRASSMANN-VALUED CONDENSATES

In this appendix we prove that Grassmann-valued condensates cannot arise. To be concrete, we consider a possible $\langle\bar{q}_s\tilde{q}_v\rangle$, where q_s is a sea quark and $\tilde{q}_v$ a ghost quark. The relevant part of the path integral is of the form[21]

$$Z^{(q)} \equiv \int\prod_{i=1}^{N} d\tilde{q}_i^* d\tilde{q}_i d\bar{q}_i dq_i \exp[-\bar{q}Xq - \bar{q}A\tilde{q} - \tilde{q}^\dagger Bq - \tilde{q}^\dagger Y\tilde{q}], \tag{A1}$$

where X corresponds to the sea-quark Dirac operator and Y to the ghost-quark Dirac operator. Here the variables q_i and $\bar{q}_i$, $i = 1, \ldots, N$, are independent Grassmann-valued (fermionic) variables, and the variables $\tilde{q}_i$ are bosonic, c-number variables. The matrices X and Y contain c-number entries, while the matrices A and B are Grassmann-valued. Of course, the matrices A and B vanish in mixed-action QCD. But, in order to study the possible occurrence of a mixed sea-ghost condensate, one chooses (appropriate entries of) A and B nonzero, and then one takes the limit of A and B to zero after the volume has been taken to infinity.

Let us first recall the standard case for which also the $\tilde{q}_i$ are fermionic.[22] An example is the formation of an Aoki condensate for two flavors of Wilson fermions. In this case we would take $X = Y$ equal to the Hermitian Wilson-Dirac operator, and we may take $A_{ij} = m_A\delta_{ij}$ and $B_{ij} = -m_B\delta_{ij}$.[23] Without loss of generality, we may assume that X has been diagonalized:

$$X_{ij} = x_i\delta_{ij}. \tag{A2}$$

We then find that

$$\sum_{i=1}^{N}\langle\bar{q}_i\tilde{q}_i\rangle^{(q)} \equiv -\frac{\partial}{\partial m_A}Z^{(q)} = -Z^{(q)}\sum_{i=1}^{N}\frac{m}{x_i^2+m^2}, \tag{A3}$$

where in the last step we took $m_A = m_B = m$ and where $\langle\ldots\rangle^{(q)}$ is the unnormalized expectation value with partition function $Z^{(q)}$. After averaging over the gauge field and taking the infinite-volume limit, followed by the limit $m \to 0$, one finds a nonvanishing condensate if and only if there is a nonzero density of near-zero modes [34], because

$$\lim_{m\to 0}\frac{m}{x^2+m^2} = \pi\delta(x). \tag{A4}$$

Now let us return to the case in which the $\tilde{q}_i$ are bosonic. The entries of A and B are now fermionic, and we can, in fact, use this to work out what happens in any basis. Taking $A_{ij} = \alpha\delta_{ii_0}\delta_{jj_0}$ for some fixed values of i_0 and j_0, the integral (A1) now evaluates to

$$\begin{aligned} Z^{(q)} &= \mathrm{sdet}\begin{pmatrix} X & A \\ B & Y \end{pmatrix} = \det(X - AY^{-1}B)/\det(Y) \\ &= \det(X)\exp(-\mathrm{tr}(X^{-1}AY^{-1}B))/\det(Y) \\ &= \det(X)(1 - \mathrm{tr}(X^{-1}AY^{-1}B))/\det(Y), \end{aligned} \tag{A5}$$

and we find (taking Grassmann derivatives to be left derivatives)

$$\frac{\partial Z^{(q)}}{\partial\alpha} = -(Y^{-1}BX^{-1})_{j_0i_0}\det(X)/\det(Y). \tag{A6}$$

It is clear that in this case, in contrast to the standard case reviewed above, no nonvanishing value can occur for a Grassmann-valued condensate in the limit that $B \to 0$. The basic reason is that we can always expand the condensate in terms of the components of A and B, resulting in a finite polynomial in those components. When we take A and B to zero, the corresponding Grassmann-valued condensates will thus always vanish. We conclude that when we consider the vacuum expectation value for the field Σ in Eq. (2.1), we can set $\omega = \bar{\omega} = 0$.

Two more comments are appropriate. First, one might wonder what would happen if one takes the matrices A and B to be bosonic. In this case, $Q = \bar{q}A\tilde{q} + \tilde{q}^\dagger Bq$ is Grassmann-valued, and it is easy to see, by expanding the exponent in Eq. (A1) in terms of Q, that in this case the partition function does not depend on A and B at all. Condensates would thus trivially vanish.

Our second comment is that the same question can also be studied in ChPT. In other words, one can assume that *a priori* ω and $\bar{\omega}$ in Eq. (2.1) do not vanish. One then finds that the equations of motion (for constant fields) in the effective theory dictate that ω and $\bar{\omega}$ vanish. This is, of course, consistent with the QCD-based argument given above.

APPENDIX B: PROOF OF EQ. (3.5)

Consider the matrix [cf. Eq. (3.4)]

$$\Sigma_q = \begin{pmatrix} \Sigma_{ss} & i\Sigma_{sv} \\ i\Sigma_{vs} & \Sigma_{vv} \end{pmatrix}, \tag{B1}$$

where all the entries on the right-hand side are two-by-two matrices with complex entries. As we have seen, Σ_q is

[21] The argument for the vanishing of $\langle\bar{q}_v\tilde{q}_v\rangle$, with q_v a valence quark, is similar, except that in this case $X = Y$.

[22] In that case, the $q_i^\dagger$, like the $\bar{q}_i$, are independent fermionic variables as well.

[23] For $m_A = m_B$ this corresponds to an Aoki condensate pointing in the σ_2 direction in isospin space.

an element of SU(4). The unitarity constraint $\Sigma_q\Sigma_q^\dagger = \mathbf{1}$ provides constraints on the submatrices:

$$\Sigma_{ss}\Sigma_{ss}^\dagger + \Sigma_{sv}\Sigma_{sv}^\dagger = \mathbf{1}, \tag{B2a}$$

$$\Sigma_{vs}\Sigma_{vs}^\dagger + \Sigma_{vv}\Sigma_{vv}^\dagger = \mathbf{1}, \tag{B2b}$$

$$\Sigma_{sv}\Sigma_{vv}^\dagger = \Sigma_{ss}\Sigma_{vs}^\dagger. \tag{B2c}$$

The effective theory is invariant under independent flavor rotations in the sea and the valence sector. With $V_s \in U(2)_{\rm sea}$ and $V_v \in U(2)_{\rm val}$, Σ_q transforms into

$$\Sigma_q' = \begin{pmatrix} V_s\Sigma_{ss}V_s^\dagger & iV_s\Sigma_{sv}V_v^\dagger \\ iV_v\Sigma_{vs}V_s^\dagger & V_v\Sigma_{vv}V_v^\dagger \end{pmatrix}. \tag{B3}$$

We now want to prove that this matrix can be brought into the form (3.5) if $\Sigma_{vv} = \rho_v\mathbf{1}$, with ρ_v an arbitrary complex number.

First, from Eq. (B2b) we conclude that

$$\Sigma_{vs} = \sqrt{1-|\rho_v|^2}C, \tag{B4}$$

where $C \in U(2)$. We also find the bound $|\rho_v| \le 1$. Equation (B2c) implies that $\Sigma_{sv}\Sigma_{vv}^\dagger\Sigma_{vv}\Sigma_{sv}^\dagger = \Sigma_{ss}\Sigma_{vs}^\dagger\Sigma_{vs}\Sigma_{ss}^\dagger$, and hence

$$|\rho_v|^2\Sigma_{sv}\Sigma_{sv}^\dagger = (1-|\rho_v|^2)\Sigma_{ss}\Sigma_{ss}^\dagger. \tag{B5}$$

Substituting this into Eq. (B2a), we obtain $\Sigma_{ss}\Sigma_{ss}^\dagger = \Sigma_{vv}\Sigma_{vv}^\dagger = |\rho_v|^2$, and we may thus write Σ_{ss} as

$$\Sigma_{ss} = \rho_v^* A, \tag{B6}$$

where $A \in U(2)$. From Eq. (B5) we obtain $\Sigma_{sv} = \sqrt{1-|\rho_v|^2}B$, with, from Eq. (B2c), $B = AC^\dagger$. Performing a flavor transformation with $V_v = C^\dagger$, we can thus write Σ_q as

$$\Sigma_q = \begin{pmatrix} \rho_v^* A & i\rho_v^\perp A \\ i\rho_v^\perp \mathbf{1} & \rho_v\mathbf{1} \end{pmatrix}, \tag{B7}$$

where we introduced $\rho_v^\perp = \sqrt{1-|\rho_v|^2}$.

The matrix A can be written as $\exp(i\alpha_\mu\tau^\mu)$, where $\tau^\mu = (\mathbf{1}, \vec{\tau})$. Hence we can define $U = \exp(-i\alpha_\mu\tau^\mu/2)$, with $AU^2 = 1$. Performing a flavor rotation with $V_s = U$ and writing $U^\dagger = e^{i\phi}V$ with $V \in SU(2)$ simplifies Σ_q to

$$\Sigma_q = e^{i\phi}\begin{pmatrix} \rho_v^* e^{i\phi}V^2 & i\rho_v^\perp V \\ i\rho_v^\perp V & \rho_v e^{-i\phi} \end{pmatrix}. \tag{B8}$$

Finally, the SU(2) matrix can be diagonalized by a flavor transformation $V_s = V_v$ such that

$$V \to D = \exp(i\theta\tau_3/2). \tag{B9}$$

Absorbing the phase $e^{-i\phi}$ into ρ_v, we arrive at

$$\Sigma_q = e^{i\phi}\begin{pmatrix} \rho_v^* D^2 & i\rho_v^\perp D \\ i\rho_v^\perp D & \rho_v \end{pmatrix}. \tag{B10}$$

This is precisely Eq. (3.5). Because $\Sigma_q \in SU(4)$, it follows that $\det(\Sigma_q) = e^{4i\phi} = 1$ and thus that $\phi = 0 \bmod \pi/2$.

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