

Effective theory for quenched lattice QCD and the Aoki phase

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(Received 16 March 2005; published 12 May 2005)

We discuss the symmetries of quenched QCD with Wilson fermions, starting from its Lagrangian formulation, taking into account the constraints needed for convergence of the ghost-quark functional integral. We construct the corresponding chiral effective Lagrangian, including terms linear and quadratic in the lattice spacing. This allows us to study the phase structure of the quenched theory, and compare it to that in the unquenched theory. In particular we study whether there may be an Aoki phase (with parity and flavor spontaneously broken) or a first-order transition line (with no symmetry breaking but meson masses proportional to the lattice spacing), which are the two possibilities in the unquenched theory. The presence of such phase structure, and the concomitant long-range correlations, has important implications for numerical studies using both quenched and dynamical overlap and domain-wall fermions. We argue that the phase structure is qualitatively the same as in the unquenched theory, with the choice between the two possibilities depending on the sign of a parameter in the low-energy effective theory.

DOI: 10.1103/PhysRevD.71.094503

PACS numbers: 12.38.Gc, 11.15.Ha

I. INTRODUCTION

Wilson fermions are one of the oldest and most important methods for formulating the quark sector of QCD on a lattice [1]. Not only have they (or improved versions) been used directly for many numerical computations, but they also play an important role in the more recent domain-wall [2,3] and overlap [4] formulations of lattice QCD.

Wilson fermions do not preserve the chiral symmetry of continuum QCD, and as a consequence the quark mass has to be tuned to recover chiral symmetry in the continuum limit [5]. Flavor and parity are exactly preserved, but, as observed by Aoki [6], these symmetries may be spontaneously broken by a pionic condensate for certain values of the bare quark mass. This leads to the existence of the so-called Aoki phase. In the theory with two flavors, a pionic condensate (which we can choose to point in the 3-direction in isospin space) breaks the $SU(2)$ of isospin down to $U(1)$, giving rise to two Goldstone bosons at nonzero lattice spacing. Within the Aoki phase, the third pion has a mass proportional to a , the lattice spacing. In the continuum limit, the Aoki phase shrinks to zero width, the pions all become massless, and the pionic condensate can be rotated (by a nonsinglet axial transformation) into the usual condensate associated with spontaneous chiral symmetry breaking.

The existence of the Aoki phase was investigated by two of us [7] using the chiral effective Lagrangian for pions in

two-flavor unquenched lattice QCD (see also Ref. [8]). It was found that indeed an Aoki phase may occur near the continuum limit, if a certain low-energy constant in the effective Lagrangian has a particular sign. For the other choice of sign, however, there was no spontaneous breakdown of flavor and parity, but rather a first-order transition, in the vicinity of which the three degenerate pions have masses proportional to a .

In this paper we attempt to extend the effective Lagrangian investigation of Ref. [7] to the quenched theory. We have several motivations for doing so. First, the issue is theoretically interesting, and challenging, because of the presence of ghost quarks in the Lagrangian formulation of quenched QCD. While the peculiarities and pathologies of the quenched theory do show up in perturbative investigations of the effective theory [9,10], they are more prominent in the nonperturbative analysis needed to study the phase structure.¹

Second, the issue is of practical importance for domain-wall and overlap fermions. Both are built upon the (Hermitian) Wilson-Dirac operator with a large negative quark mass. This operator is effectively quenched (even in dynamical domain-wall or overlap simulations) because its quark mass is not related to that of the physical quarks. As explained in detail in Ref. [11], the negative quark mass

¹We recognize that the quenched theory is not a thermodynamic system in the usual sense, as the quarks do not influence the gluon fields. Nevertheless, the properties of quarks propagating on quenched gluon fields as a function of the bare quark mass exhibit the nonanalyticities familiar from thermodynamics, so we think it appropriate to use the term “phase structure.”

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must be chosen so that one does not lie in or near any Aoki phase. The arguments of Ref. [11] also imply that, if there is a first order transition like that of the unquenched theory, one should not simulate near the phase transition line. The essential point is to avoid regions where the quenched pion correlators are long ranged. Thus it is clearly important to understand the phase structure of the quenched theory.

Finally, numerical simulations provide some evidence for the presence of the Aoki phase in the quenched theory [12]. Indeed, results from quenched simulations led Aoki to make his original proposal of a new phase.²

More recent work has shown, however, that the situation in the quenched theory is different from, and more subtle than, that in the unquenched theory. In particular, it was observed (see, for example, Ref. [14]) that there always appears to be a nonvanishing density of near-zero modes of the (Hermitian) Wilson-Dirac operator in quenched QCD if the quark mass is in the supercritical region.³ This implies a nonvanishing pionic condensate, and thus, through the Banks-Casher relation [15], would seem to lead to the conclusion that an Aoki phase fills the whole supercritical region, in contrast to what is expected in unquenched QCD. It was shown in Ref. [11] that this is not the case, however, if one defines the Aoki phase as that region of the phase diagram where Goldstone bosons associated with the symmetry breaking occur. To see this, Ref. [11] considered quenched QCD with two flavors in the presence of a twisted quark mass, which explicitly breaks flavor and parity symmetry. It was argued that (in the limit of vanishing twisted quark mass) regions may exist where the condensate does not vanish because of the existence of a density of exponentially localized near-zero modes, without any of the corresponding long-range physics usually associated with spontaneous symmetry breaking. This phenomenon is an artifact of the quenched approximation, and was shown to be consistent with the usual Ward-identity argument for the existence of Goldstone bosons. It turns out that, in the quenched case only, the Ward identity can be satisfied without a Goldstone pole even in the presence of a nonvanishing condensate, if this condensate arises because of localized near-zero modes [11]. Since the localization length of these near-zero modes is of order the lattice spacing, this phenomenon leaves no trace in the long-distance behavior of the quenched theory.

The implication of the analysis of Ref. [11] is that, in the quenched theory, there is not a one-to-one relation between the pionic condensate in an effective field theory (which is sensitive only to long-distance physics) and that determined on the lattice. While a prediction of a nonzero pionic

condensate in the effective field theory implies the presence of a lattice pionic condensate, the converse is not true. Thus numerical evidence of a condensate is not, by itself, pertinent to the question of the phase structure. What is pertinent, however, is the presence of a region in the phase diagram in which there are long-distance correlation lengths, i.e. pion masses satisfying $m_\pi \ll \Lambda_{\text{QCD}}$. An effective low-energy theory can be used in any such region. A considerable body of numerical evidence indicates that the quenched pion mass does extrapolate to very small values. Based on this, we assume that there is a region where an effective theory can be used, and then study its properties.

To carry out such a study we need a quenched effective Lagrangian that is suited to nonperturbative investigations. A systematic approach to the quenched theory along the lines of the continuum development of Ref. [16] was given in Ref. [9]. It turns out, however, that, while this approach is sufficient for setting up chiral perturbation theory (ChPT), the effective Lagrangian given in [9] is not suitable for the study of the phase structure of the theory.

In the approach of Ref. [9], a ghost quark is introduced for every valence quark [17]. The ghost quarks couple to the gluons in the same way as the valence quarks, and have the same mass, spin, and flavor symmetries. The only difference is that ghost quarks have bosonic statistics. Their determinant cancels that from the valence quarks, thus providing a path-integral definition of quenched QCD. (For the extension to the case with both valence and sea quarks, see Ref. [18].) The ghost sector was dealt with only formally in Ref. [9], without regard to the convergence of the ghost-quark path integral. Since the ghosts are bosonic, this is a nontrivial issue. While the formal treatment of Ref. [9] is sufficient to develop quenched ChPT [19], a more careful treatment leads to a somewhat different symmetry structure of the quenched QCD Lagrangian [20]. This different symmetry structure leads to a different chiral Lagrangian, which, while equivalent to the one of Ref. [9] for ChPT, is also suitable for nonperturbative investigations. The construction of this Lagrangian and its use to investigate the Aoki phase for the two-flavor theory are the central subjects of this paper.

We should stress at the outset that our analysis is, in several respects, incomplete. At various stages we are forced to make additional assumptions not required in the corresponding analysis of the unquenched theory. While we think our assumptions are reasonable, it would clearly be preferable to avoid them.

The plan of the paper is as follows. In Sect. II we define quenched QCD with N flavors of Wilson fermions, paying careful attention to the convergence of the ghost-quark path integral. In order to do this, we formulate the theory in Euclidean space, as is done in numerical simulations. In Sect. III we discuss the symmetries of this theory in detail, and then use these in Sect. IV to construct the chiral

²In the unquenched theory, recent simulations suggest, however, that, with the Wilson gauge action, the scenario with a first-order phase transition applies [13].

³Defined as the region where the bare quark mass satisfies $-8r < ma < 0$. This is where the Wilson-Dirac operator can, in principle, have exact zero modes.

effective Lagrangian both in the continuum limit and including the leading effects of discretization. In Sect. V we employ the resulting effective potential, as well as certain general properties of the quenched theory and the large- N_c limit (N_c is the number of colors), to analyze the two-flavor theory. We end with a summary and some concluding remarks. An appendix briefly reviews illustrative calculations of quenched small-volume partition functions. A preliminary account of this work was given in Ref. [21].

II. N-FLAVOR QUENCHED QCD WITH WILSON FERMIONS

In order to define quenched QCD, we introduce, for every physical quark field q , a ghost-quark field \tilde{q} with the same quantum numbers (spin, flavor, and color) as q but opposite statistics [17]. If there are N flavors, both q and \tilde{q} are N -dimensional vectors in flavor space. In the continuum, the Euclidean Lagrangian for quenched QCD may then be defined as

$$\begin{aligned} \mathcal{L} = & \bar{q}_L D q_L + \bar{q}_R D q_R + \bar{q}_R M q_L + \bar{q}_L \bar{M} + \tilde{q}_R^\dagger D \tilde{q}_L \\ & + \tilde{q}_L^\dagger D \tilde{q}_R + \tilde{q}_L^\dagger M \tilde{q}_L + \tilde{q}_R^\dagger \bar{M} \tilde{q}_R, \end{aligned} \quad (1)$$

where

$$q_L = P_L q, \quad q_R = P_R q, \quad \bar{q}_L = \bar{q} P_R, \quad \bar{q}_R = \bar{q} P_L, \quad (2)$$

in accordance with standard conventions, while, in the ghost sector,

$$\tilde{q}_L = P_L \tilde{q}, \quad \tilde{q}_R = P_R \tilde{q}, \quad \tilde{q}_L^\dagger = \tilde{q}^\dagger P_L, \quad \tilde{q}_R^\dagger = \tilde{q}^\dagger P_R. \quad (3)$$

Our convention is $P_{L,R} = (1 \pm \gamma_5)/2$. We take the mass matrices to satisfy $\bar{M} = M^\dagger$; numerical simulations usually involve real diagonal mass matrices, with $M = M^\dagger = \bar{M}$.

In Euclidean space, the Grassmann variables $q_{R,L}$ and $\bar{q}_{L,R}$ are all independent, and the integration over them leads to the quark partition function which is just the determinant of the fermionic operator,

$$\det(D + M P_L + \bar{M} P_R). \quad (4)$$

This result holds for arbitrary mass matrices M and \bar{M} . For the integral over the bosonic ghost fields to converge, however, we must restrict M and \bar{M} to be Hermitian with all eigenvalues positive. (The Euclidean Dirac operator D is anti-Hermitian, and thus plays no role in the convergence.) Since we are taking $\bar{M} = M^\dagger$, this means that $M = \bar{M}$. The Gaussian integral then leads to the ghost-quark partition function

$$\det^{-1}(D + M P_L + \bar{M} P_R) = \det^{-1}(D + M). \quad (5)$$

This cancels the quark determinant, and we see that indeed Eq. (1) describes quenched QCD. We stress that $\tilde{q}_{R,L}^\dagger$ must be the Hermitian conjugates of $q_{R,L}$ for the integral over ghost fields to converge, while no such connection exists

between q and \bar{q} . These facts will have implications for the symmetries of quenched QCD, to be discussed in the next section.

We would like to extend this continuum (and thus still formal) definition to lattice QCD with Wilson fermions. In the lattice action, D is replaced by the naive (nearest-neighbor) lattice discretization, which retains the anti-Hermiticity of the continuum D . The mass term M is replaced by $M + W$, where M is a local lattice mass term and W the Wilson term,

$$\begin{aligned} (\bar{q}_R W q_L)(x) = & -\frac{1}{2} \sum_{\mu} \bar{q}_R(x) r(U_{\mu}(x) q_L(x + \mu) \\ & + U_{\mu}^\dagger(x - \mu) q_L(x - \mu) - 2q_L(x)). \end{aligned} \quad (6)$$

The corresponding term with $L \leftrightarrow R$, which we call \bar{W} , contains \bar{r} . In general we need to take r and \bar{r} to be flavor matrices, so that we can treat them as spurion fields. They will always be related by $\bar{r} = r^\dagger$. In simulations, however, one usually takes $r = \bar{r}$ to be the identity matrix, and this is the choice we make for the remainder of this section.

As is well known, in order to approach the chiral limit at nonzero lattice spacing one must work at negative bare quark mass. This is necessary because W , being positive semidefinite, makes a positive contribution to the physical quark mass. But once the quark mass is negative, so that M has negative eigenvalues, there are some configurations on which $D + M + W$ itself can have eigenvalues with a negative or vanishing real part. (The case of vanishing real part corresponds to the so-called ‘‘exceptional configurations.’’) It follows that we cannot simply take over the definition (1), with $M \rightarrow M + W$, to define the quenched lattice theory, since the ghost-quark integral would be ill-defined. The same holds true in the continuum if M has negative eigenvalues.

In these cases we must proceed in a different way. We begin with the unquenched quark Lagrangian for Wilson fermions with $M = \bar{M}$, and we work in a basis in which the mass matrix M is diagonal, while adding an infinitesimal parity-odd mass term:

$$\mathcal{L}_{\text{quark}} = \sum_{j=1}^N [\bar{q}'_j (D + M_j + W) q'_j - \epsilon_j \bar{q}'_j i \gamma_5 q'_j]. \quad (7)$$

Here j is the flavor index, and the infinitesimal parameters ϵ_j can have either sign independently for each flavor. We use primed fields in Eq. (7) because, in order to avoid the problem of nonpositive eigenvalues of $D + M + W$, we perform a change of variables given by the following axial transformation:

$$\begin{aligned} q'_j &= \exp\left[\text{sgn}(\epsilon_j) i \frac{\pi}{4} \gamma_5\right] q_j, \\ \bar{q}'_j &= \bar{q}_j \exp\left[\text{sgn}(\epsilon_j) i \frac{\pi}{4} \gamma_5\right]. \end{aligned} \quad (8)$$

The quark-sector Lagrangian becomes

$$\mathcal{L}_{\text{quark}} = \sum_{j=1}^N [\bar{q}_j (D + \text{sgn}(\epsilon_j) i \gamma_5 (M_j + W)) q_j + |\epsilon_j| \bar{q}_j q_j]. \quad (9)$$

The resulting lattice Dirac operator $D \pm i \gamma_5 (M + W)$ is anti-Hermitian,⁴ and thus is suitable for extension to the ghost sector. Furthermore, the ϵ_j terms (which, after the axial transformation, look like regular mass terms) ensure convergence once we extend to the ghost sector. Note that for this to be true the direction of the axial rotation in Eq. (8) must be correlated with the sign of the infinitesimal parity-odd mass term in Eq. (7).

We can now define quenched lattice QCD with Wilson fermions by adding the ghost sector:

$$\mathcal{L}_W = \sum_{j=1}^N [\bar{q}_j (D + \text{sgn}(\epsilon_j) i \gamma_5 (M_j + W)) q_j + \tilde{q}_j^\dagger (D + \text{sgn}(\epsilon_j) i \gamma_5 (M_j + W)) \tilde{q}_j + |\epsilon_j| (\bar{q}_j q_j + \tilde{q}_j^\dagger \tilde{q}_j)]. \quad (10)$$

Because of the exceptional configurations mentioned above, quenched correlation functions diverge, in general, in the limit $\epsilon_j \rightarrow 0$, since zero modes of $D + M + W$ are also, after the axial rotation, zero modes of $D \pm i \gamma_5 (M + W)$ [22]. We therefore keep the ϵ_j nonzero, but infinitesimal.

Several comments are in order. First, one may worry that the transformation of Eq. (8) could be anomalous. This is not the case. The fermionic measure on the lattice is rigorously invariant, and no vacuum angle θ is generated. This is in accordance with the fact that in order to produce a nonzero vacuum angle from Wilson fermions, one has to introduce a relative phase between the Wilson mass (W) and the single-site mass (M) [23].⁵

Second, the fact that the sign of ϵ_j may be chosen independently for each quark flavor has interesting consequences. For example, with two quenched flavors, one may choose $\epsilon \equiv \epsilon_u = -\epsilon_d > 0$ for the up and down flavors. This corresponds to (quenched) twisted-mass lattice QCD [6,25]. It leads, after the axial transformation, to the Lagrangian

$$\mathcal{L}_W^{2\text{-flavor}} = \bar{q} (D + i \tau_3 \gamma_5 (M + W)) q + \tilde{q}^\dagger (D + i \tau_3 \gamma_5 (M + W)) \tilde{q} + \epsilon (\bar{q} q + \tilde{q}^\dagger \tilde{q}), \quad (11)$$

where τ_3 is the diagonal Pauli matrix acting in flavor space. We see that, in order to guarantee convergence of the

⁴This form is unfamiliar, but is, in fact, unitarily equivalent to i times the well-known Hermitian Wilson-Dirac operator, $H_W = \gamma_5 [D \pm (M + W)]$.

⁵See Ref. [24] for an alternative method.

ghost-quark integral, a nontrivial flavor dependence is introduced into the quark-mass and Wilson terms. If we choose ϵ_u and ϵ_d of the same sign, however, no such flavor dependence appears. We will analyze both cases in this paper.

For later use, we rewrite the Lagrangian (10) in two other ways. For the sake of clarity we give the expressions only for the simplest choice of the ϵ_j , namely, that all are equal and positive: $\epsilon_j = \epsilon > 0$. It is straightforward to generalize the expressions to any other choice for the ϵ_j by going back to Eq. (10). We first rewrite \mathcal{L}_W in terms of the γ_5 projected fields of Eqs. (2) and (3):

$$\mathcal{L}_W = \bar{q}_L D q_L + \bar{q}_R D q_R + \bar{q}_R \tilde{M} q_L + \bar{q}_L \tilde{M}^\dagger q_R + \tilde{q}_R^\dagger D \tilde{q}_L + \tilde{q}_L^\dagger D \tilde{q}_R + \tilde{q}_L^\dagger \tilde{M} \tilde{q}_L + \tilde{q}_R^\dagger \tilde{M}^\dagger \tilde{q}_R, \quad (12)$$

with $\tilde{M} = i(M + W - i\epsilon)$, and ϵ implicitly multiplied by the identity matrix in flavor space. Next, we group the quark and ghost-quark fields into a ‘‘super field’’

$$\Psi_{L,R} = \begin{pmatrix} q_{L,R} \\ \tilde{q}_{L,R} \end{pmatrix}, \quad \bar{\Psi}_{R,L} = \begin{pmatrix} \bar{q}_{R,L} & \tilde{q}_{L,R}^\dagger \end{pmatrix}, \quad (13)$$

in terms of which

$$\mathcal{L}_W = \bar{\Psi}_L D \Psi_L + \bar{\Psi}_R D \Psi_R + \bar{\Psi}_R \mathcal{M} \Psi_L + \bar{\Psi}_L \overline{\mathcal{M}} \Psi_R, \quad (14)$$

with

$$\mathcal{M} = i \begin{pmatrix} M + W - i\epsilon & 0 \\ 0 & M + W - i\epsilon \end{pmatrix}, \quad (15)$$

and $\overline{\mathcal{M}} = \mathcal{M}^\dagger$.

III. SYMMETRIES OF CONTINUUM QUENCHED QCD

In this section we consider the symmetries of quenched QCD in the continuum limit. In that limit, the Wilson term is irrelevant once the additive renormalization of the quark mass has been included. Thus we can treat the quantity $M + W$ as simply a quark-mass matrix. Note that, because of our use of the axial transformation (8), we can treat the quenched theory for either sign of the quark masses.

It is instructive to first discuss the quark and ghost sectors separately. For $\tilde{M} = 0$, the quark part of \mathcal{L}_W is invariant under

$$q_{L,R} \rightarrow V_{L,R} q_{L,R}, \quad \bar{q}_{L,R} \rightarrow \bar{q}_{L,R} V_{L,R}^{-1}, \quad (16)$$

with V_L and V_R both elements of $GL(N)$ (for N flavors). Thus the chiral symmetry group is $GL(N)_L \times GL(N)_R$. (This ignores the anomaly, to which we return below.) This can be maintained as a symmetry of the full quark Lagrangian if \tilde{M} and \tilde{M}^\dagger are treated as *independent* spurion fields. Renaming the latter as $\tilde{M}^\dagger \rightarrow \overline{\tilde{M}}$, the required transformations are

$$\tilde{M} \rightarrow V_R \tilde{M} V_L^{-1}, \quad \overline{\tilde{M}} \rightarrow V_L \overline{\tilde{M}} V_R^{-1}. \quad (17)$$

We take the vector subgroup to be that which remains when M and r are proportional to the identity matrix and all ϵ_j are equal. This requires $V_L = V_R$, so that the vector subgroup is the diagonal subgroup $GL(N)$.

The symmetry group of the quark sector in the Euclidean formulation is larger than that of the Hamiltonian formulation, where the group $GL(N)$ is reduced to the unitary group $U(N)$. It is straightforward to show that the larger group (which is just the complexification of $U(N)$) does not lead to any new Ward identities (see for instance Ref. [19]).

In the ghost sector, the symmetry transformations of \tilde{q}_L and \tilde{q}_R are coupled, and, setting $\tilde{M} = 0$ in Eq. (12), the ghost Lagrangian is invariant under [20]

$$\tilde{q}_L \rightarrow V \tilde{q}_L, \quad \tilde{q}_R \rightarrow V^{\dagger-1} \tilde{q}_R, \quad (18)$$

with $V \in GL(N)$. In other words, if $\tilde{q}_{L,R} \rightarrow V_{L,R} \tilde{q}_{L,R}$, the form of the ghost Lagrangian leads to the requirement that

$$V_L = V_R^{\dagger-1} \equiv V. \quad (19)$$

The transformations of the spurion fields \tilde{M} and $\overline{\tilde{M}}$ are

$$\tilde{M} \rightarrow V^{\dagger-1} \tilde{M} V^{-1}, \quad \overline{\tilde{M}} \rightarrow V \overline{\tilde{M}} V^{\dagger}. \quad (20)$$

The vector subgroup, which we define as the subgroup which leaves $\tilde{q}_L^{\dagger} \tilde{q}_L$ and $\tilde{q}_R^{\dagger} \tilde{q}_R$ invariant, has $V^{\dagger} V = 1$, i.e. $V \in U(N)$. If we parametrize $V \in GL(N)$ as

$$V = \exp(\alpha_0 + \sum_i \alpha_i T_i), \quad (21)$$

with T_i the Hermitian generators of $SU(N)$ and $\alpha_{0,i}$ complex, then the vector subgroup has $\alpha_{0,i}$ imaginary. ‘‘Axial’’ transformations are those with α and α_i real, so that $V = V^{\dagger}$.

Next, we discuss the symmetries of the full Lagrangian, considering also transformations of quarks into ghost quarks and *vice versa*. For this, it is useful to start from the form of the Lagrangian given in Eq. (14). If Ψ and $\overline{\Psi}$ were independent, then \mathcal{L}_W would be invariant under

$$\Psi_{L,R} \rightarrow \mathcal{V}_{L,R} \Psi_{L,R}, \quad \overline{\Psi}_{L,R} \rightarrow \overline{\Psi}_{L,R} \mathcal{V}_{L,R}^{-1}, \quad (22)$$

with $\mathcal{V}_{L,R} \in GL(N|N)$, as long as we treat \mathcal{M} and $\overline{\mathcal{M}}$ as independent spurion fields transforming as

$$\mathcal{M} \rightarrow \mathcal{V}_R \mathcal{M} \mathcal{V}_L^{-1}, \quad \overline{\mathcal{M}} \rightarrow \mathcal{V}_L \overline{\mathcal{M}} \mathcal{V}_R^{-1}. \quad (23)$$

This would imply that the (massless) quenched theory possesses the graded chiral symmetry group $GL(N|N)_L \times GL(N|N)_R$. This does not take into account, however, that $\overline{\Psi}_{L,R}$, when restricted to the ghost sector, is not independent of $\Psi_{L,R}$, but rather, that

$$\overline{\Psi}_{L,R}|_{\text{ghost, body}} = \Psi_{R,L}^{\dagger}|_{\text{ghost, body}}. \quad (24)$$

What this equation means is the following. After a graded

transformation, the ghost field \tilde{q} picks up terms containing Grassmann numbers. In general, \tilde{q} can be split into its ‘‘body’’ and a ‘‘soul,’’ where the body is the usual complex field, and the soul is even in Grassmann fields or parameters. As discussed in more detail in Ref. [19], it is sufficient for the convergence of the ghost integral that Eq. (24) apply only to the body of the ghost fields, as already indicated in that equation. It can then be shown that the restriction of Eq. (19) generalizes to [19]

$$\mathcal{V}_{Lgg}|_{\text{body}} = \mathcal{V}_{Rgg}^{\dagger-1}|_{\text{body}}, \quad (25)$$

where, in $N \times N$ block form (for N flavors),

$$\mathcal{V}_L = \begin{pmatrix} \mathcal{V}_{Lqq} & \mathcal{V}_{Lqg} \\ \mathcal{V}_{Lgq} & \mathcal{V}_{Lgg} \end{pmatrix}, \quad (26)$$

and similar for \mathcal{V}_R . The label q refers to the quark sector, and the label g to the ghost sector. Note that the resulting set of transformations,

$$\mathcal{G} = \{(\mathcal{V}_L, \mathcal{V}_R) \in GL(N|N)_L \times GL(N|N)_R | \\ \times \mathcal{V}_{Lgg}|_{\text{body}} = \mathcal{V}_{Rgg}^{\dagger-1}|_{\text{body}}\}, \quad (27)$$

still forms a group.

To complete the discussion of continuous symmetries we review the impact of the anomaly [9]. In the continuum limit, transformations in \mathcal{G} for which $\text{sdet}(\mathcal{V}_L) \neq \text{sdet}(\mathcal{V}_R)$ are anomalous, and should be excluded. This can be accomplished by restricting $\mathcal{V}_{L,R}$ to lie in $SL(N|N)$ rather than $GL(N|N)$. There is one subtlety, however. The nonanomalous vector $U(1)$ transformations do not commute with general elements of $SL(N|N)$ and so the complete symmetry group is a semidirect product [26]:

$$\mathcal{G} = \{(\mathcal{V}_L, \mathcal{V}_R) \in [SL(N|N)_L \times SL(N|N)_R] \times U(1)_V | \\ \times \mathcal{V}_{Lgg}|_{\text{body}} = \mathcal{V}_{Rgg}^{\dagger-1}|_{\text{body}}\}. \quad (28)$$

The vector subgroup (the subgroup which leaves $\overline{\Psi}\Psi$ invariant) is not affected by the anomaly and is given by

$$\mathcal{H} = \{(\mathcal{V} = \mathcal{V}_L = \mathcal{V}_R) \in GL(N|N) | \\ \times \mathcal{V}_{gg}|_{\text{body}} = \mathcal{V}_{gg}^{\dagger-1}|_{\text{body}}\}. \quad (29)$$

For further discussion of the symmetry group, see Ref. [19].

Finally, we consider the properties of \mathcal{L}_W under parity. Unquenched QCD with Wilson fermions in the standard form is invariant under parity, but this is not obviously true for our definition of quenched QCD. In terms of the new quark variables of Eq. (8), a parity transformation acts on the spinor indices as

$$q(t, \vec{x}) \rightarrow i\gamma_4 \gamma_5 q(t, -\vec{x}), \quad \overline{q}(t, \vec{x}) \rightarrow \overline{q}(t, -\vec{x}) i\gamma_5 \gamma_4, \quad (30)$$

and the quark sector of \mathcal{L}_W is invariant under this transformation (if the gauge field is transformed accordingly).

The ghost sector is not, however, invariant under this symmetry. If we try to define parity on the ghost field as

$$\tilde{q}(t, \vec{x}) \rightarrow i\gamma_4\gamma_5\tilde{q}(t, -\vec{x}) \Rightarrow \tilde{q}^\dagger(t, \vec{x}) \rightarrow -\tilde{q}^\dagger(t, -\vec{x})i\gamma_5\gamma_4, \quad (31)$$

the ghost part of \mathcal{L}_W transforms into minus itself.

However, as long as we consider correlation functions involving only physical quark fields parity is not broken. Parity breaking can then only come from ghost loops, but these are always exactly cancelled by physical quark loops. A more formal version of the argument follows when we couple only the physical quarks to external sources. After integrating over the quark and ghost fields, the determinants cancel, and only the physical quark propagator couples to the sources. We conclude that parity is not broken in quenched QCD, with the proviso that we only consider correlation functions made out of physical quark fields.

It will be useful to consider also “naive” parity:

$$\begin{aligned} q(t, \vec{x}) &\rightarrow \gamma_4 q(t, -\vec{x}), & \bar{q}(t, \vec{x}) &\rightarrow \bar{q}(t, -\vec{x})\gamma_4, \\ \tilde{q}(t, \vec{x}) &\rightarrow \gamma_4\tilde{q}(t, -\vec{x}), & \tilde{q}^\dagger(t, \vec{x}) &\rightarrow \tilde{q}^\dagger(t, -\vec{x})\gamma_4. \end{aligned} \quad (32)$$

Under this transformation, the kinetic terms of both the quark and ghost sectors are invariant, but not the mass terms, which transform into minus themselves because of the γ_5 they contain. The Lagrangian (14) is, however, invariant if we transform the spurion fields \mathcal{M} and $\overline{\mathcal{M}}$ under naive parity as

$$\mathcal{M} \rightarrow \overline{\mathcal{M}}, \quad \overline{\mathcal{M}} \rightarrow \mathcal{M}. \quad (33)$$

IV. QUENCHED CHIRAL EFFECTIVE LAGRANGIAN

In this section, we discuss the construction of the effective theory for the Goldstone particles of quenched QCD, assuming that the chiral symmetry is spontaneously broken and that Goldstone-like excitations occur. These assumptions are based mainly on the results from numerical simulations. The order parameter for symmetry breaking is the quark condensate, which, for positive degenerate quark masses, is aligned so that the vector symmetry is unbroken.

We will need to address several issues that arise in the quenched theory that are not present when constructing the effective theory for unquenched QCD. The first is the fact that, in the quenched theory, a nonvanishing condensate does not necessarily lead to Goldstone-like excitations [11]. The Ward identity can be saturated by localized near-zero modes of the lattice Dirac operator. According to the conjecture of Ref. [11], such near-zero modes are present throughout the supercritical region, except where there are extended near-zero modes. In the latter case, the Ward identity is saturated by the usual Goldstone particles. The net effect of these observations is that the condensate in the chiral Lagrangian cannot be identified with that at

the quark level, but rather with a “long-distance” condensate defined by removing the contributions of short-distance near-zero modes. Since the $\epsilon_j \rightarrow 0$ divergences in quenched correlation functions are due to localized near-zero modes [11], we conjecture that the limit $\epsilon_j \rightarrow 0$ can be taken after the removal of these short-distance near-zero modes.⁶

The second issue concerns the presence of infrared divergences in the chiral limit which make this limit singular [9,10]. To avoid these, we assume that there is a region with small enough (but nonzero) quark masses for which the correlation lengths of Goldstone correlation functions are much larger than those of other excitations in the theory, so that it makes sense to use the effective Lagrangian approach.

The third issue is the need to keep the “singlet” Goldstone field, Φ_0 (defined precisely below), despite the fact that the corresponding symmetry is anomalous. This point is explained in Refs. [9,10,19]: Φ_0 must be kept in the effective theory because its correlators have long-distance contributions, even though some of these contributions are not those of a standard single-particle pole.

The remaining issues will be discussed as they arise in the rest of this section. In the first subsection we discuss the effective theory for quenched QCD in the continuum limit. In the second subsection we extend this to include terms of order a and a^2 , where a is the lattice spacing.

A. Continuum Effective Lagrangian

Here we construct the effective Lagrangian for quenched QCD in the continuum limit, starting from the formulation of quenched QCD developed in Sect. II. This was done before in Ref. [9], but there it was naively assumed that the full chiral symmetry group is the graded group $U(N|N)_L \times U(N|N)_R$, an assumption which we have seen above not to be entirely correct. It turns out that the effective Lagrangian is equivalent to that of Ref. [9] if the aim is only to develop chiral perturbation theory for quenched QCD, but not if one wants to do nonperturbative calculations, such as needed to explore the Aoki phase.

Following the standard development, we expect the Goldstone excitations to be described by a nonlinear field Σ which transforms as $\Psi_L \overline{\Psi}_R$ and spans the coset \mathcal{G}/\mathcal{H} :

$$\Sigma = \exp(\Phi), \quad \Sigma \rightarrow \mathcal{V}_L \Sigma \mathcal{V}_R^{-1}. \quad (34)$$

Here $\mathcal{V}_{L,R}$ are elements of the symmetry group \mathcal{G} , Eq. (28), and \mathcal{H} is the unbroken subgroup of Eq. (29). If $\langle \Sigma \rangle$ is proportional to the identity matrix, then Φ is a linear combination of the broken generators. To construct a Lagrangian invariant under \mathcal{G} , we also need $\Sigma^{-1} \rightarrow \mathcal{V}_R \Sigma^{-1} \mathcal{V}_L^{-1}$, transforming as $\Psi_R \overline{\Psi}_L$. As already noted above, however, we must enlarge Σ to include the

⁶In principle, this can be done by allowing only admissible gauge fields [27].

“super- η' ” field $\Phi_0 \equiv -i \text{str} \log \Sigma = -i \log \text{sdet} \Sigma$ (str is the supertrace, sdet the superdeterminant). This can be done by allowing $\mathcal{V}_{L,R}$ to be elements of the larger, anomalous, group \mathcal{G}' , Eq. (27), while still only requiring the Lagrangian to be invariant under \mathcal{G} . Since Φ_0 is invariant under \mathcal{G} , this leads to the usual presence of an arbitrary set of functions of this singlet field in the effective Lagrangian [9,16].

With these ingredients, and treating the masses as spurions as described above, the $O(p^2)$ effective Lagrangian becomes

$$\begin{aligned} \mathcal{L}_{\text{eff}} = & \frac{1}{8} f^2 V_1(\Phi_0) \text{str}(\partial_\mu \Sigma \partial_\mu \Sigma^{-1}) \\ & - v V_2(\Phi_0) \text{str}(\mathcal{M} \Sigma + \Sigma^{-1} \overline{\mathcal{M}}) \\ & + \frac{1}{2} c_0 \Phi_0^2 V_0(\Phi_0) + \frac{1}{2} \alpha (\partial_\mu \Phi_0)^2 V_5(\Phi_0), \end{aligned} \quad (35)$$

with $V_i(\Phi_0) = 1 + O(\Phi_0^2)$, $i = 0, 1, 2, 5$. We have used a field redefinition to remove possible terms linear in Φ_0 [9,16]. The constant c_0 is of $O(\Lambda^2)$ ($\Lambda \equiv \Lambda_{\text{QCD}}$ being the nonperturbative scale of QCD) and, because of its relation to the η' mass and topological susceptibility, is expected to be positive [9,10]. The mass matrix \mathcal{M} , Eq. (15), becomes (taking all ϵ_j positive and equal for simplicity) $\mathcal{M} = i(m - i\epsilon)$ with $m = M - m_c(r)$ the subtracted mass matrix,⁷ and $\overline{\mathcal{M}} = \mathcal{M}^\dagger$. The plus sign in the mass term follows from the fact that under naive parity $\Sigma \rightarrow \Sigma^{-1}$ and $\mathcal{M} \leftrightarrow \overline{\mathcal{M}}$, cf. Eq. (33). Note that, while this looks like the standard mass term in ChPT, there are factors of $\pm i$ hidden in \mathcal{M} and $\overline{\mathcal{M}}$, related to the original singlet axial field redefinition of Eq. (8).

We now consider how to parametrize the field Φ . Were it not for the restrictions on the ghost-ghost part of the transformations, Φ would generate $GL(N|N)$ and thus be a general complex graded matrix. The restriction (19) implies, however, that the ghost-ghost part of Φ must have a Hermitian body, and so we parametrize it as

$$\Phi = \begin{pmatrix} i\phi_1 + \phi_2 & \overline{\chi} \\ \chi & \hat{\phi} \end{pmatrix}, \quad (36)$$

with $\phi_{1,2}$ Hermitian $N \times N$ matrices of c -numbers, χ and $\overline{\chi}$ $N \times N$ matrices of independent Grassmann variables, and $\hat{\phi}$ a Hermitian c -number $N \times N$ matrix. Note that, in addition, $\phi_{1,2}$ as well as $\hat{\phi}$ can have arbitrary souls.

⁷ $m_c(r)$ is the critical quark mass. As one approaches the continuum limit, this can be defined as the value for which the pions become massless. This definition does not work away from the continuum limit, however, since the subsequent analysis shows that the pions may have a minimal mass of $O(a)$, or there may be a region of quark masses for which there are massless pions. For our purposes, however, it is sufficient to have a definition which determines m_c to within an accuracy of $O(a\Lambda^2)$, and one such definition is that the pion mass should be of size $a\Lambda^2$.

There are a number of unusual features of the parametrization (36). First and foremost, the presence of both ϕ_1 and ϕ_2 in Eq. (36) implies a redundancy in the number of fields describing the physical pions. This redundancy is not, however, special to the quenched theory—it occurs also in unquenched QCD. The standard prescription is to set $\phi_2 = 0$, so that Σ is unitary in the quark sector, reflecting the fact that only the unitary subgroup are symmetries of the Hamiltonian. We will follow this prescription here, and briefly review the arguments supporting this choice for the quenched theory.⁸

First, we note that the effective Lagrangian depends only on the field $\phi = \phi_1 - i\phi_2$, and not on $\phi_1 + i\phi_2$. If one is only interested in developing chiral perturbation theory one may just expand in ϕ (as well as $\hat{\phi}$, χ , and $\overline{\chi}$). This leads to the standard Feynman rules in the physical meson sector.⁹ However, if one wishes to consider nonperturbative issues such as the phase diagram of the theory, or the exact finite-volume partition function, the contour of integration of ϕ needs to be specified.

We note in passing that the absence of a factor of i multiplying $\hat{\phi}$ in (36) means that the propagator for ghost-ghost mesons has the sign of a physical meson propagator (due to the minus sign from the supertrace). This differs, superficially, from the standard Feynman rules of quenched chiral perturbation theory in which the ghost-ghost mesons have wrong sign propagators [9]. There are also, however, additional factors of i in vertices, and it is straightforward to see that these factors can be shuffled from vertices to propagators in such a way as to reproduce the standard rules. This is why the use of the correct symmetry group is unnecessary when only developing perturbation theory. Of course, in order to see the relation to standard quenched chiral perturbation theory one must also “undo” axial rotations of Eq. (8).

A stronger argument for setting $\phi_2 = 0$ is that, if we choose to integrate the field ϕ along the contour $\phi_2 = 0$, the quenched small-volume partition function is independent of the quark mass, as it should be [28,29].¹⁰ A different contour would not lead to the same result. In the Appendix we give a demonstration of this in the one-flavor theory in the sector with zero topological charge, using a parametrization which makes the calculation particularly simple.

Another feature of the parametrization (36) is the presence of the “souls” (nilpotent parts) of the fields ϕ_1 , ϕ_2 , and $\hat{\phi}$. In particular, the soul of $\hat{\phi}$ need not be Hermitian, although the body must be. As discussed in Ref. [19],

⁸For a parallel discussion in the partially quenched case see Ref. [19].

⁹In fact, we are assuming implicitly in this discussion that we should use the Lagrangian (37) as is, rather than taking its real part. We are also assuming that the parameters f , v , etc. are real.

¹⁰Here “small-volume” refers to the regime $m_\pi L \ll 1 \ll \Lambda_{\text{QCD}} L$, with L the linear size of the volume.

however, the souls do not contribute to integrals, as long as the integrals are convergent. Thus, in effect, we can treat ϕ_1 , ϕ_2 , and $\hat{\phi}$ as standard Hermitian matrices, with the prescription discussed above setting $\phi_2 = 0$.

One might be concerned that if we restrict the degrees of freedom in Σ by setting $\phi_2 = 0$, and thus reduce the set of allowed transformations of Σ , we might have to allow additional terms to appear in the effective Lagrangian. We suspect that, in fact, the correct approach is to use the full symmetries to determine the effective Lagrangian, and then restrict the manifold of Σ . If so, this would remove the concern. But, in any case, the remaining transformations are sufficient to forbid additional terms. These transformations are unitary in the quark-quark block, Hermitian in the ghost-ghost block, and arbitrary in the quark-ghost blocks.

B. Order a Effects

In this section, we consider how the flavor-symmetry structure of quenched QCD with Wilson fermions is modified at nonvanishing lattice spacing. From now on, we will always choose all physical and ghost-quark masses equal to m . In the unquenched case, it was argued in Ref. [7] that the relevant continuum quark Lagrangian including terms of order a (the lattice spacing) is given by

$$\begin{aligned} \mathcal{L}_{\text{quark,eff}} = & \mathcal{L}_{\text{gluons}} + \bar{q}(D + i\gamma_5 m)q \\ & + a\bar{q}b_1 i\gamma_5 i\sigma_{\mu\nu} F_{\mu\nu} q + O(a^2), \end{aligned} \quad (37)$$

with b_1 a coefficient which depends on the QCD coupling constant. The term linear in a is the Pauli term. The matrix $i\gamma_5$ appears in both the mass and Pauli terms because of the field redefinition Eq. (8). The Pauli term breaks chiral symmetry in the same way as the mass term, and this symmetry breaking may thus be represented by a spurion field A which transforms just as \tilde{M} in Eq. (17).

In the quenched case, analogous arguments lead to the quark effective Lagrangian

$$\begin{aligned} \mathcal{L}_{\text{quark,eff}}^{\text{quenched}} = & \mathcal{L}_{\text{gluons}} + \bar{\Psi}(D + i\gamma_5 m)\Psi \\ & + a\bar{\Psi}b_1 i\gamma_5 i\sigma_{\mu\nu} F_{\mu\nu} \Psi + \epsilon\bar{\Psi}\Psi + O(a^2), \end{aligned} \quad (38)$$

where b_1 can take a different value in the quenched case. We have included the convergence term, taking $\epsilon_j = \epsilon > 0$ for all flavors. Note that the effective Dirac operator $D + i\gamma_5 m - b_1 a\gamma_5 \sigma_{\mu\nu} F_{\mu\nu}$ is anti-Hermitian, as is the corresponding operator in the underlying lattice theory.

The extra $i\gamma_5$ appears in the mass and Pauli terms because of the unusual form (30) that parity takes in our formulation of quenched QCD. In fact, the situation is somewhat subtle. Parity is broken in the ghost sector (cf. Sect. III), and indeed, the ghost part of the Pauli term as well as that of the mass term in Eq. (38) breaks parity: like

the rest of the ghost Lagrangian, it changes sign under (31). However, as already observed at the end of Sect. III, if we restrict ourselves to consider only correlation functions involving physical quark fields, parity is not broken by the underlying lattice theory, and correspondingly also not by $\mathcal{L}_{\text{quark,eff}}^{\text{quenched}}$. A term of the form $\bar{\Psi}\sigma_{\mu\nu}F_{\mu\nu}\Psi$ cannot appear, because it would break parity in the physical sector. Under naive parity (cf. Eq. (32)) the Pauli terms also switch sign, just like the mass terms.

It follows that, as in the unquenched theory, the Pauli term breaks chiral symmetry in the same way as the mass term. We may introduce spurion fields $\mathcal{A} = ib_1$, $\bar{\mathcal{A}} = -ib_1 = \mathcal{A}^\dagger$ transforming just like \mathcal{M} and $\bar{\mathcal{M}}$ in Eq. (23) to keep track of this symmetry breaking at the level of the Goldstone-meson effective Lagrangian.

With this new spurion field, we can extend the effective Lagrangian of Eq. (35) to include $O(a)$ effects. The rule is simply that every appearance of \mathcal{M} could be replaced by \mathcal{A} . We are interested in vacuum structure and so will consider only the potential. We keep all terms of size m^2 , ma , and a^2 — $O(p^4)$ in the usual chiral counting. Recalling that all masses are degenerate, we find

$$\begin{aligned} V(\Sigma) = & -ic_1 \text{str}(\Sigma - \Sigma^{-1}) - \epsilon \text{str}(\Sigma + \Sigma^{-1}) + \frac{1}{2}c_0\Phi_0^2 \\ & + c_2((\text{str}\Sigma)^2 + (\text{str}\Sigma^{-1})^2) + c_3(\text{str}\Sigma)(\text{str}\Sigma^{-1}) \\ & + c_4(\text{str}(\Sigma^2) + \text{str}(\Sigma^{-2})), \end{aligned} \quad (39)$$

with

$$\begin{aligned} c_1 = & \alpha_1 m\Lambda^3 + \alpha_2 a\Lambda^5, \\ c_2 = & \beta_1 m^2\Lambda^2 + \beta_2 ma\Lambda^4 + \beta_3 a^2\Lambda^6, \\ c_3 = & \gamma_1 m^2\Lambda^2 + \gamma_2 ma\Lambda^4 + \gamma_3 a^2\Lambda^6, \\ c_4 = & \delta_1 m^2\Lambda^2 + \delta_2 ma\Lambda^4 + \delta_3 a^2\Lambda^6, \end{aligned} \quad (40)$$

Here α_i , β_i , γ_i , and δ_i are dimensionless constants of order one, and the factors of Λ are as required by dimensional analysis. The c_i terms in (39) can also be multiplied by Φ_0 dependent potentials, but we do not make this explicit since we will argue in the next section that we can set $\Phi_0 = 0$ in the vacuum.

There is an apparent inconsistency in our analysis. We have kept $O(a^2)$ terms in the effective Lagrangian, but not in the underlying quark Lagrangian, $\mathcal{L}_{\text{quark,eff}}^{\text{quenched}}$. The missing terms (e.g. four-fermion operators) do not, however, break any further symmetries and so do not lead to additional terms in $V(\Sigma)$. The only exception is a three derivative term $\sim \bar{\Psi}\gamma_\mu D_\mu^3 \Psi$, which breaks the rotation group down to its hypercubic subgroup, but this maps into a term with four derivatives in the effective chiral Lagrangian, and is thus absent from $V(\Sigma)$.

Finally, we address the issue of the relative size of the coefficient c_1 and the coefficients $c_{2,3,4}$. Following Ref. [7], we distinguish three regimes:

- (1) The quark mass is physical while $a \rightarrow 0$. This means m/Λ is a (small) constant, so that, for $a \rightarrow 0$, $c_{2,3,4} \sim \frac{m}{\Lambda} c_1$ are small compared to c_1 . Both lattice artifacts and the contributions of $O(m^2)$ terms can be ignored. In this case $c_1 \propto m$, a result we use several times below. In fact, the proportionality constant ($\alpha_1 \Lambda^2$) is very likely to be positive,¹¹ and we phrase subsequent discussions as though this is true, although our final conclusions would not change if α_1 were negative.
- (2) The quark mass is $O(a)$ itself, i.e. $am \sim (a\Lambda)^2$. In this case, $c_{2,3,4}$ are still small compared to c_1 , but the $O(a)$ term in c_1 cannot be ignored. The critical value of m is shifted by an amount $\sim a\Lambda^2$, and one may define m' as a subtracted quark mass such that the pion mass vanishes at $m' = 0$. The two terms in c_1 are both of the same order.
- (3) The subtracted quark mass is of order $am' \sim (a\Lambda)^3$. In this case, we have that $c_1 \sim m'/\Lambda^3$ and $c_{2,3,4} \sim a^2 \Lambda^6 \sim c_1$. In other words, for this case the higher-order terms in $V(\Sigma)$ compete with the lower-order term, and we need to consider both to determine the vacuum structure of the theory. As already observed in Ref. [7], this leads to the prediction that the width of a potential Aoki phase is of order a^3 (for small a). In this regime, higher-order terms beyond those shown in Eq. (39) are of higher order in a , and therefore need not be included in the analysis [7].

In summary, the quenched approximation has introduced several new features to the potential: traces have become supertraces; there are three $O(p^4)$ terms in the potential rather than one, due to the different group structure; there are extra terms involving Φ_0 ; and, finally, the requirement to do an axial rotation has led to the leading masslike term having the form $\Sigma - \Sigma^{-1}$ rather than $\Sigma + \Sigma^{-1}$. We now turn to the question of how these changes influence the phase diagram.

V. PHASE DIAGRAM

We now address the central question of this paper, whether there can be an Aoki phase in the quenched theory, analogous to that predicted for the unquenched two-flavor theory. This might seem to be just a matter of minimizing the potential we have constructed, but there are a number of subtleties in the ghost sector that complicate the analysis. In fact, we will need certain additional properties of the

quenched theory, which we collect before proceeding to the full analysis.

A. Additional Properties of the Quenched Theory

To study the spontaneous breaking of parity and the flavor-symmetry group \mathcal{H} of Eq. (29), we will only allow source terms which respect the graded symmetry between a quark and its corresponding ghost quark. The reason is, of course, that ghost quarks are not present in numerical simulations, but instead the quark determinant is simply omitted. The ghost-quark is just a field-theoretical trick to describe this procedure in terms of a path integral, and our choice of sources should be restricted accordingly. Furthermore, it is sufficient to use source terms which are diagonal in flavor. This is because we can choose any flavor-breaking condensate to point in the τ_3 direction. The fact that the source terms are flavor-diagonal then implies that quarks of different flavors are not coupled (either by the action or the sources). This in turn means that quenched correlation functions involving only one flavor of quark depend only on the mass of that quark, and not on those of other quarks, or even their presence or absence. It also follows that correlation functions involving ghost quarks are identical, up to a possible overall sign, to those for the corresponding quark, since they are composed of the same propagators. These results hold for any lattice spacing and thus also in the continuum limit.

A consequence of these observations is that the quenched condensate for each flavor is independent of the number of flavors, and that any ghost condensate is equal to that of the corresponding quark. This holds not only for the bare lattice condensates, but also for the physical condensates. The latter are obtained by subtracting divergent contributions from the bare condensate, and then multiplying by a matching factor. These steps maybe difficult to implement in practice, but what matters to us here is that they can be done in principle, and that the subtractions and matching factors do not depend on the number or properties of flavors other than that in the condensate itself. It follows, in particular, that any spontaneous symmetry breaking pattern does not break symmetries in \mathcal{H} such that any ghost-quark condensate would be different from the corresponding quark condensate.

Our next observation concerns the quenched condensate in the continuum limit. In this limit, one can ignore the b_1 term in Eq. (38), and the quark condensate is an odd function of the quark mass, configuration by configuration:

$$\begin{aligned} \text{tr}[1/(D + i\gamma_5 m)] &= \text{tr}[\gamma_3^2/(D + i\gamma_5 m)] \\ &= -\text{tr}[1/(D - i\gamma_5 m)]. \end{aligned} \quad (41)$$

If the condensate has a nonvanishing nonperturbative contribution, as we are assuming, then this too must be odd in m . The same holds for the corresponding ghost-quark condensate. Such a behavior is indeed seen in numerical

¹¹In the unquenched theory α_1 (which is related to the Gasser-Leutwyler parameter B_0) is known to be positive, and we do not expect quenching to change the sign of this parameter. Numerical evidence supports this expectation.

results for the quenched condensate with staggered and overlap fermions, which is odd under $m \rightarrow -m$. At the level of the effective chiral Lagrangian, working in the continuum limit means that $c_1 \propto m$ and $c_{2,3,4} \propto m^2$ in Eq. (39), and the result (41) implies that Σ_{qq} (the component of the condensate for quark q), and the corresponding ghost condensate Σ_{gg} , should, in the continuum limit, both change sign when c_1 does. This result also follows from symmetries in the following somewhat indirect way. First, for the condensate in the physical sector, Σ_{qq} , this can be derived using the appropriate axial symmetry in order to flip the sign of m . Then, because of the arguments given above, the corresponding ghost condensate, Σ_{gg} , has to follow suit. We note that there is no “direct” way of changing the sign of m in the ghost sector, as follows from Eq. (20). We note also that this result does not hold in the unquenched theory because the measure depends on the quark mass.

In light of the previous discussion, one might wonder why we need to consider more than one flavor in the quenched theory. The reason we need two flavors is to allow the calculation of flavor nonsinglet pion propagators. These have only quark-connected contributions and are the quantities usually calculated in simulations. It is the masses of these pions which are observed to extrapolate to zero at nonzero lattice spacing—the phenomenon which the Aoki phase was introduced to explain. With one flavor alone one can only consider flavor-singlet pions, which have quark-disconnected contributions as well.

We also need to recall some properties of the quenched theory in the limit that N_c , the number of colors, becomes large.¹² In the continuum effective Lagrangian, Eq. (35), standard arguments show that the constants f^2 and ν are proportional to N_c , while c_0 and α are $O(1)$. The latter two are suppressed because they multiply terms corresponding to disconnected diagrams at the quark level. Similarly, in the potential for nonzero lattice spacing, Eq. (39), the coefficients of the single-supertrace terms, c_1 (which is proportional to νm), and c_4 , are $O(N_c)$, while the coefficients of terms with two supertraces, c_0 , c_2 , and c_3 , are $O(1)$. Thus in the large- N_c limit we can set c_0 , c_2 , and c_3 to zero.

The advantage of this limit is, of course, that the quark sector becomes physical, since the quark determinant is suppressed by $1/N_c$. In other words, there is no distinction between quenched and unquenched theories in this limit. Thus the results of our analysis of the quenched theory must, in the quark sector, coincide with those of the unquenched two-flavor theory in this limit. The analysis of the Aoki phase in the unquenched theory in the large- N_c

limit is a simple generalization of that at finite N_c [7]. In particular, the competition between two contributions which leads to the nontrivial phase structure remains in the large- N_c limit (since these are the c_1 and c_4 terms). The only significant change is that the flavor group $SU(2)$ is enlarged to $U(2)$. This larger symmetry group may then be broken down to $U(1) \times U(1)$ (as opposed to a single $U(1)$) in the Aoki phase, so there are still two exact Goldstone bosons. Further details will be discussed below.

The particular utility of the large- N_c limit is that it allows us to check our method of analysis of the ghost sector. We have argued above that, with sources appropriately chosen, the quark and ghost condensates must be the same. Since the analysis in the quark sector becomes unquenched as $N_c \rightarrow \infty$, this means that we know the result which we must obtain in the ghost sector in this limit.

B. Phase Diagram as $N_c \rightarrow \infty$

We start from the effective potential $V(\Sigma)$ of Eq. (39) for two flavors, u and d , and substitute the form for Φ , Eq. (36). In fact, we can simplify this form as follows: first, by setting $\chi = \bar{\chi} = 0$, since these are the solutions of the classical equations of motion for these fields; second, by setting $\phi_2 = 0$, as discussed in the previous section; and, third, by keeping only flavor-diagonal components of the fields since we force any flavor-breaking to lie in the τ_3 direction. Thus we can investigate the vacuum structure using an expectation value

$$\langle \Sigma \rangle \equiv \Sigma = \text{diag}(e^{i\phi_u}, e^{i\phi_d}, e^{\hat{\phi}_u}, e^{\hat{\phi}_d}), \quad (42)$$

where $-\pi < \phi_{u,d} \leq \pi$ are real phases, while $\hat{\phi}_{u,d}$ are real variables to be integrated along the entire real axis.

In this subsection we consider the large- N_c limit, and thus set $c_0 = c_2 = c_3 = 0$. The potential is then

$$\begin{aligned} V = 2 \sum_{j=u,d} & [\text{sgn}(\epsilon_j) c_1 \sin(\phi_j) - |\epsilon_j| \cos(\phi_j)] \\ & + c_4 \cos(2\phi_j) + i \text{sgn}(\epsilon_j) c_1 \sinh(\hat{\phi}_j) \\ & + |\epsilon_j| \cosh(\hat{\phi}_j) - c_4 \cosh(2\hat{\phi}_j). \end{aligned} \quad (43)$$

Here we have reintroduced the dependence on the ϵ_j , which follows from the fact that the lattice mass and Wilson terms in Eq. (10) are proportional to $\text{sgn}(\epsilon_j)$. The c_4 term does not depend on the sign of ϵ_j since it is quadratic in symmetry breaking. The factorization into four parts, dependent, respectively, on ϕ_u , ϕ_d , $\hat{\phi}_u$, and $\hat{\phi}_d$, is the result of taking $N_c \rightarrow \infty$. This is how, in this context, the quark and ghost sectors decouple.

In the quark sectors the analysis is essentially a recapitulation of that of Ref. [7] for the unquenched two-flavor theory, except that here it is done for each flavor separately. The notation is also different: our c_4 was called $-c_2/4$ in

¹²One subtlety of this limit is that we must take $N_c \rightarrow \infty$ before $m \rightarrow 0$, so that the quenched artifacts proportional to $\ln(m)/N_c$ vanish. Since we are implicitly working at small but nonvanishing quark masses, so as to avoid these artifacts, we are able to take the large- N_c limit without problems.

Ref. [7], and here we have done an axial transformation which complicates the interpretation of the condensate. What remains unchanged is the region of parameters of interest: c_1 is proportional to the $O(a)$ shifted quark mass m' while $c_4 \sim a^2$ is a constant. A useful ratio is $\eta = c_1/4c_4$. We want to determine what happens to the condensate as η ranges from values smaller than -1 to larger than 1 , in the limit $\epsilon \rightarrow 0$. We note that the term proportional to $|\epsilon_j|$ can be dropped for most of the analysis, since we take $\epsilon_j \rightarrow 0$ at the end, except where it is needed to distinguish between otherwise degenerate minima.

It is useful, first, to consider the continuum theory in which $c_4 = 0$, so that the potential in each quark sector is $V_q = 2\text{sgn}(\epsilon_q)c_1 \sin(\phi_q)$, where we now use an index q instead of j to indicate that we are considering the quark sector of a given flavor q . For positive c_1 (corresponding to positive quark mass in the original basis) the minimum is at $\phi_q = -\text{sgn}(\epsilon_q)\pi/2$, so that $\Sigma_{qq} = e^{i\phi_q} = -\text{sgn}(\epsilon_q)i$. For negative c_1 , the minimum switches to $\phi_q = \text{sgn}(\epsilon_q)\pi/2$, so that $\Sigma_{qq} = \text{sgn}(\epsilon_q)i$. In short, the minimum occurs at $\Sigma_{qq} = -\text{sgn}(\epsilon_q c_1)i$. This reproduces the standard discontinuous dependence of the direction of the condensate as a function of the direction of the mass and source terms.

The unusual factor of $-i$ in the condensate is a reflection of the axial transformation Eq. (8) needed to define the quenched theory. If we rotate back to the usual continuum basis, then the condensate becomes $\Sigma_{qq} = \text{sgn}(c_1)$. In other words the nonstandard values of ϕ_q undo the axial transformation. To see this explicitly, we can write the potential in terms of shifted fields $\phi_q = -\text{sgn}(\epsilon_q c_1)\pi/2 + \phi'$:

$$\begin{aligned} V_q &= -2|c_1| \cos \phi' - 2c_4 \cos 2\phi' \\ &= -2(|c_1| + c_4) + (|c_1| + 4c_4)\phi'^2 + O(\phi'^4), \end{aligned} \quad (44)$$

where we have restored the c_4 term in anticipation of the discussion below. This is the potential we would have obtained directly if we had not had to use the trick with the axial transformation of Eq. (8), and instead expanded about $\Sigma_{qq} = \pm 1$.

Now we consider nonvanishing c_4 . If $c_4 > 0$, the analysis with $c_4 = 0$ goes through unchanged: the $c_4 \cos(2\phi_q)$ term has equal minima at $\phi_q = \mp \pi/2$, so it is the sign of $\epsilon_q c_1$ which determines the direction of the condensate. There is thus a first-order transition when c_1 changes sign.

If $c_4 < 0$, however, it contributes negative curvature to V_q , which can destabilize the minima. Looking at the quadratic terms in Eq. (44), we see that this happens when $4c_4 < -|c_1|$, i.e. $|\eta| < 1$. The minimum of the potential shifts to $\phi_q = \text{sgn}(\epsilon_q) \arcsin(\eta)$, signaling that we are in an Aoki phase. There are two choices of branch for the inverse sine, one interpolating between $-\pi/2$ and

$+\pi/2$, the other between $-\pi/2$ and $-3\pi/2$. In both cases the condensate “swings” from $-i$ to $+i$ around the unit circle in the complex plane, when $\epsilon_q c_1$ changes from positive to negative values. The choice of branch decides which way the condensate swings, i.e. whether it passes through $+1$ or -1 when $\eta = c_1 = 0$. Which choice is appropriate is determined by the $|\epsilon_j|$ term in Eq. (43). This term is negative if $-\pi/2 < \phi_q < \pi/2$ and positive if $-3\pi/2 < \phi_q < -\pi/2$, and thus selects the branch in which Σ_{qq} swings through $+1$. This is true irrespective of the sign of ϵ_j .

The symmetry that is broken by the condensate depends on the details of the theory. If we were considering one flavor alone, then, undoing the axial transformation (8), we would find that $\langle \bar{q}i\gamma_5 q \rangle \propto \text{sgn}(\epsilon_q)\sqrt{1-\eta^2} \neq 0$ for $|\eta| < 1$. Thus parity is broken in the Aoki phase. The sign of the condensate is determined by the sign of $\epsilon_q \equiv \epsilon_j$ in Eq. (7). There are no exact Goldstone bosons in this phase as no continuous lattice symmetry is broken.

Next, we consider the two-flavor theory, with degenerate masses. The pattern of symmetry breaking depends on the signs we choose for ϵ_u and ϵ_d in Eq. (7). If we choose ϵ_u and ϵ_d both of the same sign, so that Eq. (7) represents a flavor-singlet source proportional to $\sum_q \bar{q}i\gamma_5 q$, then the condensates will satisfy $\langle \bar{u}i\gamma_5 u \rangle = \langle \bar{d}i\gamma_5 d \rangle \neq 0$, and parity, but not flavor, will be broken (so again there are no Goldstone bosons). We checked explicitly, from Eq. (39) with $c_0 = c_2 = c_3 = 0$, that in this case indeed there are no Goldstone bosons (all pions have a mass of order a). If, on the other hand, we use a flavor-breaking source term proportional to $\bar{u}i\gamma_5 u - \bar{d}i\gamma_5 d$ (i.e. $\epsilon_d = -\epsilon_u$), the mass term in the lattice quark Lagrangian will be proportional to τ_3 (cf. Eq. (11)), which translates into the c_1 terms in Eq. (43) for the up and down sectors having opposite signs. The condensates will then satisfy $\langle \bar{u}i\gamma_5 u \rangle = -\langle \bar{d}i\gamma_5 d \rangle \neq 0$, and flavor and parity will be broken. This is the most familiar example of the Aoki phase, which has two Goldstone bosons π^\pm , and which carries over to finite N_c in the unquenched theory (see Sect. VC below). In this case, the calculation of the meson spectrum from the chiral Lagrangian is virtually identical to that in Ref. [7], and confirms the existence of two massless Goldstone bosons. We stress, however, that, as far as the condensate is concerned, these theories at infinite N_c differ only kinematically—the underlying phenomenon is identical in all cases.

We now turn to the ghost sector, in which the potential is

$$V_g = 2[ic'_1 \sinh(\hat{\phi}) + |\epsilon| \cosh(\hat{\phi}) - c_4 \cosh(2\hat{\phi})]. \quad (45)$$

We have dropped the index j because, in the remainder of this section, we are only interested in demonstrating that, for each flavor, the ghost sector follows the quark sector.

We have introduced the useful variable¹³ $c'_1 \equiv \text{sgn}(\epsilon_j)c_1$. As in the quark sector, we can ignore the $|\epsilon|$ term except when it breaks degeneracies.

The potential (45) is complex, and the usual approach of minimizing it to find the vacuum structure breaks down. However, what one is really doing if one minimizes the potential in the context of Euclidean field theory is to calculate the leading term in a saddle-point expansion of the path integral. Stating the problem this way, it is clear that this can also be done when the integrand is complex instead of real. The prescription is to treat $\hat{\phi}$ as complex, and deform the contour of integration so as to pass through a saddle-point. The vacuum expectation value of the field is, at leading order, the value at the position of the saddle. If there are multiple saddles, the appropriate one to use is determined by the boundary conditions on the contours, and other considerations, as will be discussed below.

Another issue we must face is the convergence of integrals as $\hat{\phi} \rightarrow \pm\infty$. For instance, if $c_4 > 0$, the last term in V_g is unbounded from below in these limits. In fact, we only know the form of the potential for small fields, $|\hat{\phi}| \leq 1$. The ratio of successive terms in the chiral expansion grows exponentially when $|\hat{\phi}|$ exceeds unity (as can be seen from the relative magnitude of the c_4 and c_1 terms) rapidly overcoming any suppression in their coefficients. Thus, once $|\hat{\phi}| \sim 1$ the chiral expansion breaks down, and we do not know its behavior at large fields. In light of this, we simply assume that we can treat the integral over $\hat{\phi}$ as convergent at infinity along the real axis, and search for saddles in the region $|\hat{\phi}| \leq 1$ through which the contour can be deformed in such a way that it can be evaluated using steepest descent. Note that the same issues do not arise in the ϕ_q integrals, because there is no relative exponential growth in the terms, and because the integral runs over only a short segment (of length 2π) of the real axis.

As for the quark sector, we warm up by considering the phase structure for $c_4 = 0$, so that $V_g = 2ic'_1 \sinh(\hat{\phi})$. The saddle-point equation is

$$\cosh(\hat{\phi}) = \cosh(x)\cos(y) + i\sinh(x)\sin(y) = 0, \quad (46)$$

where we have written $\hat{\phi} = x + iy$, with x and y real. The solutions to this equation are a periodically repeating sequence along the imaginary axis, with the two nearest to the origin being at $\hat{\phi}_A = -i\pi/2$ and $\hat{\phi}_B = +i\pi/2$. These correspond to the condensate taking the values $\Sigma_{gg} = \exp(\hat{\phi}_{A,B}) = \mp i$, i.e. the same values as arose in the quark sector. The other solutions lead to the same two values of the condensate and are thus not physically distinct.

¹³We could have performed the analysis in the quark sector in terms of c'_1 as well; however, there we wanted to emphasize the explicit flavor dependence of the condensate in the Aoki phase through the signs of the ϵ_q .

Expanding about the saddles, we find

$$\begin{aligned} V_g(\hat{\phi} = \mp i\frac{\pi}{2} + \hat{\phi}') &= \pm 2c'_1 \cosh(\hat{\phi}') \\ &= \pm 2c'_1 \left[1 + \frac{\hat{\phi}'^2}{2} \right]. \end{aligned} \quad (47)$$

The criteria we use to choose the saddle are based on the direction in which $\Re V_g$ rises most steeply (which is the direction the contour should follow to have the steepest descent of $|\exp(-V_g)|$ away from the saddle), as well as the value of the potential at the saddle. The contour should pass through the saddle and then be able to join the real axis for large fields, without passing near other saddles. If there is more than one saddle point with an appropriate contour, we want to *maximize* the value of $\Re V_g$, so that the contribution to the saddle-point integral is minimized, and thus a better approximation to the (absolute) value of the full integral is obtained.¹⁴ All criteria agree in this case: if $c'_1 > 0$ then V_g is larger at $\hat{\phi}_A$, and has steepest descent in the direction of $\hat{\phi}'$ real, so that the contour can be easily deformed so as to end up on the real axis for large $\hat{\phi}'$. The other saddle has its direction of steepest descent along the imaginary axis, with the contour heading directly for saddle $\hat{\phi}_A$ and its periodic reflection. If $c'_1 < 0$, the role of the two saddles is reversed, and we must choose $\hat{\phi}_B$.

In this way, the ghost condensate is predicted to flip from $-i$ to $+i$ as c'_1 passes from positive to negative values. This is exactly the same dependence as for the quark condensate, Σ_{qq} , and is in agreement with the general arguments given in Sect. VA. That this check works out gives us confidence in our method. We note for future reference that the total potential, $V_q + V_g$, vanishes at the saddles that have been chosen.

Now we add back in a nonzero c_4 , in which case the saddle-point equation becomes

$$ic'_1 \cosh(\hat{\phi}) - 2c_4 \sinh(2\hat{\phi}) = 0. \quad (48)$$

The solutions are $\hat{\phi}_{A,B}$, defined above, and an additional saddle or saddles satisfying

$$\hat{\phi}_C : \quad \sinh(\hat{\phi}_C) = ic'_1/(4c_4) \equiv i\eta'. \quad (49)$$

The solutions of this equation (apart from periodic repetitions in the imaginary direction) are

¹⁴For a lucid description of the saddle-point method, see e.g. Ref. [30].

$$\begin{aligned}
\eta' < -1 : \quad & \hat{\phi}_{C\pm} = -i\pi/2 \pm \operatorname{arcosh}(-\eta') \\
& = \hat{\phi}_A \pm \operatorname{arcosh}(-\eta'), \\
-1 \leq \eta' \leq +1 : \quad & \hat{\phi}_C = i \arcsin \eta', \\
\eta' > 1 : \quad & \hat{\phi}_{C\pm} = i\pi/2 \pm \operatorname{arcosh} \eta' \\
& = \hat{\phi}_B \pm \operatorname{arcosh} \eta'. \tag{50}
\end{aligned}$$

Expanding V_g around these saddles we find

$$\begin{aligned}
V_g(\hat{\phi}_A + \hat{\phi}') &= 2(c'_1 + c_4) + 4c_4(\eta' + 1)\hat{\phi}'^2 + O(\hat{\phi}'^3), \\
V_g(\hat{\phi}_B + \hat{\phi}') &= 2(-c'_1 + c_4) + 4c_4(-\eta' + 1)\hat{\phi}'^2 + O(\hat{\phi}'^3), \\
V_g(\hat{\phi}_C + \hat{\phi}') &= -2c_4(1 + 2\eta'^2) + 4c_4(\eta'^2 - 1)\hat{\phi}'^2 + O(\hat{\phi}'^3). \tag{51}
\end{aligned}$$

As above, our approach will be to find the saddle for which V_g increases for real displacements (which we will refer to as “positive curvature”), since the original integral over $\hat{\phi}$ is along the real axis, and which has the largest value of the potential at the saddle. We run through the choices of parameters in turn.

We begin by considering $c_4 > 0$.

$\mathbf{c}'_1 > \mathbf{4c}_4 > \mathbf{0}$, or $\eta' > 1$: Saddles A and $C\pm$ (arrayed either side of B) have positive curvature, while B has negative curvature. There are two choices of contour: that passing through A alone, and that running through $\hat{\phi}_{C-}$, $\hat{\phi}_B$, and then $\hat{\phi}_{C+}$. We choose the former as the potential is higher at A than at $C\pm$. Furthermore, saddles $C\pm$ are outside the range of applicability of our truncated effective potential except for $\eta' \approx 1$. Thus we find the same saddle as for $c_4 = 0$.

$\mathbf{4c}_4 > \mathbf{c}'_1 > \mathbf{0}$, or $0 < \eta' < 1$: Both saddles A and B have positive curvature, while C lies on the imaginary axis between A and B and has negative curvature. Thus a contour passing through either A or B is possible. We choose that through A since it has the higher potential.

$\mathbf{4c}_4 > \mathbf{0} > \mathbf{c}'_1 > -|\mathbf{4c}_4|$, or $-1 < \eta' < 0$: The saddles are similar to the previous case, except that saddle B now has the highest potential, and so we pick the contour passing through B rather than A . In other words, when c'_1 passes through zero the saddle switches from A to B , just as in the case $c_4 = 0$.

$\mathbf{4c}_4 > \mathbf{0} > -\mathbf{4c}_4 > \mathbf{c}'_1$, or $\eta' < -1$: The situation is the reflection in the real axis of that for $c'_1 > 4c_4 > 0$. Saddles B and $C\pm$ have positive curvature, and we choose the former since it has the higher potential.

Summary for $\mathbf{c}_4 > \mathbf{0}$: The ghost condensate is unchanged from the analysis when $c_4 = 0$, and satisfies $\hat{\phi} = i\phi$ for all c'_1 . Thus $\Sigma_{qq} = \Sigma_{gg}$, as expected. In both quark and ghost sectors there is a first-order phase transition as c'_1 passes through zero, just as in the continuum limit. There is no Aoki phase in either sector. The spectrum of fluctuations about both quark and ghost vacua is the same for all c'_1 .

We now turn to the case $c_4 < 0$.

$\mathbf{c}'_1 > \mathbf{4|c}_4| > \mathbf{0} > \mathbf{4c}_4$, or $\eta' < -1$: Changing the sign of c_4 changes the sign of the curvature about all saddles. Thus, in this parameter range, only saddle A has positive curvature. The contour must pass through A , and then move back to the real axis. It can do so by passing through $C\pm$ and then moving off in an imaginary direction, although this is not necessary. In all cases the integral is dominated by the value at saddle A .

$\mathbf{4|c}_4| > |\mathbf{c}'_1|; \mathbf{0} > \mathbf{c}_4$, or $|\eta'| < 1$: The contour must pass through saddle C , since this is the only saddle with positive curvature. This gives an expectation value $\hat{\phi} = i \arcsin \eta' = i \operatorname{sgn}(\epsilon_j) \arcsin \eta$, which is consistent with the equality $\hat{\phi} = i\phi$, since we found above that $\phi_q = \operatorname{sgn}(\epsilon_j) \arcsin \eta$. As for the quark sector, however, there is a choice of branch of the inverse sine function. The appropriate choice is determined by the $2|\epsilon_j| \cosh \hat{\phi}$ term in V_g : one should pick the branch which *maximizes* this term. It is easy to see that the resulting branch is that which satisfies the equality $\hat{\phi} = i\phi$ for either sign of ϵ_j , i.e. that the ghost condensate is always equal to the quark condensate.

$\mathbf{0} > \mathbf{4c}_4 > \mathbf{c}'_1$, or $\eta' > 1$: The contour passes through B , which is the only saddle with positive curvature.

Summary for $\mathbf{c}_4 < \mathbf{0}$: As for $c_4 > 0$, these results are consistent with those from the quark sector and give $\Sigma_{gg} = \Sigma_{qq}$. In particular, we find an Aoki phase in both quark and ghost sectors.

In summary, we see how the saddle-point analysis effectively restores the quark-ghost symmetry which had been broken by the need for convergence of the ghost integral.

C. Phase Diagram for Finite N_c

We now extend our analysis of the quenched phase diagram to finite N_c . Finite- N_c corrections will change the values of c_1 and c_4 , but, more importantly, turn on c_0 , c_2 , and c_3 . The latter terms couple the quark and ghost sectors, as well as the different flavors. To make progress here we will need to use the assumption, discussed in Sect. VA, that the condensates in the quark and ghost sectors have to be equal, as well as other general considerations.

We note first that it is straightforward to show that the solutions we found in Sect. VB are still solutions of the full saddle-point equations which follow from Eqs. (39) and (42). The full saddle-point equations in the finite- N_c case are transcendental equations, due to the c_0 term in the effective potential $V(\Sigma)$, and we do not know whether any solutions to these equations other than those discussed in the previous section exist. However, in the previous section we found that the ghost and quark condensates were always equal in the $N_c \rightarrow \infty$ limit, and, in accordance with the argument at the quark level in Sect. VA, we will insist that this continues to hold for finite N_c . This means

that we require $\hat{\phi}_q = i\phi_q$ for each flavor q . Remarkably, upon imposing this constraint we find that the terms proportional to c_0 , c_2 , and c_3 drop out of the saddle-point equations, and the solutions are those found in Sect. V B. Note that a similar argument applies to the terms of order Φ_0^2 and beyond¹⁵ in the potentials $V_{0,2}(\Phi_0)$ in Eq. (35).

We conclude that reducing N_c from infinity does not change the saddles we need to consider. This is the good news. The bad news is that, since we are now considering the coupled $\phi_q, \hat{\phi}_q$ system, we must use the full potential when distinguishing between the saddles, and, as noted above, this potential vanishes for all of them.

To make progress, we consider in general the role of the $c_0\Phi_0^2$ term in the quenched chiral potential (39). A signature result of quenched chiral perturbation theory is that, at tree level, this term does not shift the position of the pole in the flavor-singlet propagator but rather gives rise to a double-pole contribution at the same position. This double-pole term represents the presence of quark-disconnected contributions (the so-called ‘‘double hairpins’’) in this channel [9,10].¹⁶ Furthermore, the c_0 term does not affect the value of the condensate at tree level, but rather only at one-loop through long-distance effects. This is very different from the effect of such a term in the unquenched theory. There it shifts the position of the η' pole, and changes the value of the condensate at leading order (since η' loop effects are short distance they lead to an $O(1)$ correction to the condensate proportional to $v \times M_{\eta'}^2/(4\pi f_\pi)^2$).

We conjecture that these perturbative results hold also nonperturbatively, and that the c_0 term does not influence the value of the condensate. A similar discussion applies to c_2 and c_3 terms in the potential, which both have two supertraces, and at leading order in a field expansion are proportional to Φ_0^2 . Given this conjecture, the analysis for finite N_c collapses to that for infinite N_c , and we conclude that the possible phase structures in the quenched theory at finite N_c are the same as those in the unquenched theory at infinite N_c .

We illustrate the argument for the irrelevance of c_0 , c_2 , and c_3 by studying the small fluctuations around one of the saddles. For simplicity, assume that $c'_1 > 0$ and that $c'_1 + 4c_4 > 0$ as well, so that we are in the phase with $i\phi_q = \hat{\phi}_q = -i\pi/2$ (this is saddle point A in the ghost sector). Expanding the effective potential around this saddle to quadratic order gives

$$V(\Sigma) = \frac{1}{2} \begin{pmatrix} \phi_q & \hat{\phi}_q \end{pmatrix} [2(c'_1 + 4c_4)\mathbf{I} + (c_0 + 4c_2 + 2c_3)\mathbf{X}] \times \begin{pmatrix} \phi_q \\ \hat{\phi}_q \end{pmatrix}, \quad (52)$$

¹⁵These terms all vanish in the large- N_c limit.

¹⁶We expect this to be true inside the Aoki phase as well.

in which \mathbf{I} is the unit matrix and \mathbf{X} is a matrix filled with 1's in the quark sector (upper left-hand block), i 's in the mixed quark-ghost sector, and -1 's in the ghost sector (lower right-hand block). Note that the coefficient of \mathbf{I} reproduces the coefficients of the quadratic terms in the first line of Eq. (51), as well as Eq. (44) for the case at hand.

First, ignoring \mathbf{X} , we see that the potential is stable around our solution if $c'_1 + 4c_4 > 0$, with an instability developing when $c'_1 + 4c_4 < 0$, signaling spontaneous symmetry breaking. This confirms what we found in Sect. V B. As long as $c'_1 + 4c_4 > 0$, ϕ_q and $\hat{\phi}_q$ mesons propagate with masses proportional to $c'_1 + 4c_4$.

Now if we include \mathbf{X} , the (zero-momentum) propagator can be determined from the inverse of the matrix in Eq. (52). Because $\mathbf{X}^2 = 0$, this inverse is equal to

$$\frac{1}{2(c'_1 + 4c_4)} \mathbf{I} - \frac{c_0 + 4c_2 + 2c_3}{4(c'_1 + 4c_4)^2} \mathbf{X}. \quad (55)$$

This shows that the parameters $c_{0,2,3}$ do not affect the meson masses, but instead determine the residue of the quenched double pole, which originates in the so-called ‘‘double-hairpin’’ diagram. While this double pole exhibits a sickness of the quenched theory, it does not affect the meson masses. Spontaneous symmetry breaking only occurs when the squares of these masses turn negative.

This brings us to our final point of this section, which is the effect of the flavor-singlet pseudoscalar in the unquenched theory. For simplicity we discuss only the two-flavor theory. In the unquenched theory, the flavor-singlet mass term is $(1/2)c_0\Phi_0^2 = (1/2)c_0(\phi_u + \phi_d)^2$. In the limit of vanishing $\epsilon_{u,d}$ this term raises the energy of the solution for which $\phi_u = \phi_d$. Thus, in the unquenched theory, one finds that $\langle \bar{u}i\gamma_5 u \rangle = -\langle \bar{d}i\gamma_5 d \rangle \neq 0$ inside the Aoki phase, and flavor is always broken along with parity. As we have seen, this mechanism for picking the vacuum is not present in the quenched theory. In the quenched theory, for both infinite and finite N_c , the pattern of symmetry breaking depends on the relative sign of ϵ_u and ϵ_d .

VI. CONCLUSION

The aim of this paper is to see whether the method of Ref. [7], based on the effective theory describing the Goldstone-boson physics of full QCD with two flavors of Wilson fermions, can be extended to the quenched theory. Our conclusion is that it can, although to push through the analysis we have had to make a number of assumptions not needed in the unquenched theory. We find the same two possibilities for the phase structure as in the unquenched case: depending on the sign of a parameter of the effective theory (c_4), there is either an Aoki phase or a first-order phase transition.

The nature of the quenched Aoki phase, if there is one, can however differ from that in the unquenched theory. In particular, the form of the condensate in the two-flavor

quenched theory depends on the source employed to probe spontaneous symmetry breaking. One can have a phase in which both parity and flavor symmetry are broken, as in Aoki's original scenario, but one can also have only breaking of parity, with no breaking of flavor, and thus no Goldstone bosons. Since in the quenched theory quark correlators are only probing the theory, while not being part of the dynamics (there are no sea quarks), this is a kinematical effect. For more detail, we refer to Sect. VB. Unquenched QCD at $N_c = \infty$ shares this property, but there the degeneracy between the two possibilities is lifted at finite N_c , in accordance with Ref. [7].

The extension of the method of Ref. [7] to the quenched theory turned out to be nontrivial. The formal definition of quenched QCD of Ref. [9] does not lead to a convergent path integral in the ghost sector. While expanding the Lagrangian of Ref. [9] around $\Sigma = 1$ leads to the correct version of quenched ChPT, it breaks down nonperturbatively. We gave a nonperturbatively valid path-integral definition of quenched QCD, and analyzed its symmetries. This has been discussed before in the continuum in Ref. [20], but here we extended this to lattice QCD with Wilson fermions, thus providing a fully-regulated, convergent path-integral definition of quenched QCD. We then used it to construct an effective potential to next-to-leading order, including terms up to order a^2 . Employing this effective action, we argued that the analysis of the phase structure of unquenched QCD with two Wilson fermions of Ref. [7] carries over to the quenched case. As a by-product we saw how standard quenched chiral perturbation theory is recovered.

As discussed in some more detail in Sect. VB, for certain values of the coefficients, the effective potential can be unbounded from below for large values of the fields. While the vacuum structure we found satisfies local stability, this would seem to cast a doubt on our conclusions. We believe that this problem is spurious. As we argued, the effective theory is only valid below the typical hadronic scale, and should thus not be trusted for large values of the fields. In fact, we expect that it is possible to construct a different effective potential with the same vacuum structure and the same perturbative expansion, but which is bounded for large values of the fields [31].

Finally, we remark that the entire analysis was carried out in Euclidean space. This is the relevant setting: quenching is only employed in the Euclidean version of lattice QCD. It is interesting to note that, while the Euclidean ghost action is invariant under $SO(4)$ rotations, the Minkowski version would not be invariant under Lorentz transformations, because in the ghost sector the option of identifying \bar{q} with $q^\dagger \gamma^0$ does not exist. Like with parity, this would not affect quenched correlation functions with only physical (and no ghost) quark fields on the external legs. However, we doubt that it will be possible even in principle to continue the quenched theory to Minkowski space.

ACKNOWLEDGMENTS

We thank Yigal Shamir for extensive discussions and comments on the manuscript. We also thank Carleton Detar and Jeff Greensite for comments and discussions. M. G. and R. S. thank the Department of Physics and the Institute for Nuclear Theory at the University of Washington for hospitality. M. G. also thanks the Theory and Applied Physics Divisions (T-8 and X-7) at Los Alamos National Lab for hospitality. S. R. S. thanks the School of Physics and Astronomy at the University of Southampton for hospitality. All three of us are supported in part by the US Department of Energy.

APPENDIX

First, we calculate the small-volume partition function for the one-flavor quenched theory in the sector with topological charge zero. The latter condition implies that the constant $c_0 = 0$. We include this appendix only for pedagogical reasons; for other cases as well as references, see, for example, Refs. [28,29]. In a small volume (often referred to as the “ ϵ -regime”), the dominant contribution comes from the constant modes. The partition function we wish to calculate is

$$Z(m, J) = \int_R \omega \exp \left\{ -v V \text{str} \left[\begin{pmatrix} m+J & 0 \\ 0 & m \end{pmatrix} (\Sigma + \Sigma^{-1}) \right] \right\},$$

$$\Sigma = \begin{pmatrix} A & C \\ D & B \end{pmatrix} \Rightarrow \Sigma^{-1} = \begin{pmatrix} \frac{1}{A} + \frac{CD}{A^2 B} & -\frac{C}{AB} \\ -\frac{D}{AB} & \frac{1}{B} - \frac{CD}{AB^2} \end{pmatrix}, \quad (\text{A1})$$

where V is the four-dimensional volume, and the fields are constant. A and B represent c -number degrees of freedom, while C and D represent Grassmann degrees of freedom. The integration measure $2\pi i \omega = -dA dB dC dD$ is obtained starting from the Haar measure on $GL(1|1)$, and thus, following our arguments in Sect. IVA, we restrict the bosonic part of the integration region to $R = S_1 \times R^+$ [28]. In other words, A lies on the unit circle S_1 and B lies on the positive real axis R^+ . We took the masses in the physical and ghost sectors $m+J$ and m different; the quenched theory is obtained by setting $J = 0$.

A convenient parametrization for the nonlinear field Σ equivalent to that used in the text is given by choosing

$$A = e^{i\phi'}, \quad B = e^{\hat{\phi}'}. \quad (\text{A2})$$

The relation between this parametrization and that of Eq. (36) can be worked out order by order by an expansion in the fields. (This expansion is finite, because of the Grassmann nature of the fields χ , $\bar{\chi}$, C , and D .) The advantage of our new parametrization is that the Jacobian which appears when we actually calculate the integral is simpler.

The Jacobian for the transition from A, B to $\phi', \hat{\phi}'$ is equal to $iAB = ie^{i\phi'+\hat{\phi}'}$. Expanding in C and D and defin-

ing $r = 2vVm$, $s = 2vVJ$, we find that

$$\begin{aligned} Z(m, J) &= -\frac{1}{2\pi i} \int_{-\pi}^{\pi} d\phi' \int_{-\infty}^{\infty} d\hat{\phi}' \int dC dD (iAB) \exp\left\{\frac{1}{2}(r+s)(A+1/A) - \frac{1}{2}r(B+1/B)\right\} \left[1 + \frac{CD}{2AB} \left(\frac{r+s}{A} + \frac{r}{B}\right)\right] \\ &= \frac{1}{4\pi} \int_{-\pi}^{\pi} d\phi' \int_{-\infty}^{\infty} d\hat{\phi}' \{(r+s)\cos\phi' + r\cosh\hat{\phi}'\} \exp\{(r+s)\cos\phi' - r\cosh\hat{\phi}'\} \\ &= (r+s)I_1(r+s)K_0(r) + rI_0(r+s)K_1(r). \end{aligned} \quad (\text{A3})$$

To obtain the quenched result we set $s = 0$ and find that $Z(m, 0) = 1$, irrespective of the value of m .¹⁷ This would not have been true if we had chosen A to lie on R^+ , which corresponds to choosing $\phi_1 = 0$ instead of $\phi_2 = 0$ in Eq. (36).

In the case with more than one flavor, there is more than one way to define the vectorlike subgroup \mathcal{H} of Eq. (29). For instance, for the two-flavor case, if we have a mass matrix proportional to τ_3 , it is natural to define the vectorlike subgroup in the ghost sector by requiring that V is τ_3 -Hermitian:

$$V^\dagger \tau_3 V = \tau_3, \quad (\text{A4})$$

and likewise, that $V_L = \tau_3 V_R \tau_3$ in the quark sector. The relevant group integral for the standard quenched two-flavor case, analogous to the one-flavor case reviewed above, was done in Ref. [32], and here we discuss only how things change if one chooses vectorlike transformations in the ghost sector to be τ_3 -Hermitian.

First, let us consider the parametrization of the bosonic ghost block of Σ , i.e. B of Eq. (A2) above for the two-flavor case. In Ref. [32], the following parametrization was chosen (showing only bosonic parameters, i.e. setting Grassmann parameters equal to zero)¹⁸:

$$B = e^{s_1 + s_2} \begin{pmatrix} \cosh\Phi e^{s_1 - s_2} & i \sinh\Phi e^{i\sigma} \\ i \sinh\Phi e^{-i\sigma} & \cosh\Phi e^{-(s_1 - s_2)} \end{pmatrix}. \quad (\text{A5})$$

This can be written as

$$B = e^{(\hat{\phi}_0 + \tau_3 \hat{\phi}_3)/2} e^{\tau_1 \hat{\phi}_1 + \tau_2 \hat{\phi}_2} e^{(\hat{\phi}_0 + \tau_3 \hat{\phi}_3)/2}, \quad (\text{A6})$$

with

$$\begin{aligned} s_1 + s_2 &= \hat{\phi}_0, & s_1 - s_2 &= \hat{\phi}_3, & \Phi &= \sqrt{\hat{\phi}_1^2 + \hat{\phi}_2^2}, \\ \sin\sigma &= -\frac{\hat{\phi}_1}{\Phi}, & \cos\sigma &= -\frac{\hat{\phi}_2}{\Phi}. \end{aligned} \quad (\text{A7})$$

This parametrizes the coset $GL(2)/U(2)$ for the standard choice of \mathcal{H} . For our new definition of \mathcal{H} , the relevant coset is instead parametrized by

$$B_{\tau_3} = e^{(\hat{\phi}_0 + \tau_3 \hat{\phi}_3)/2} e^{i\tau_1 \hat{\phi}_1 + i\tau_2 \hat{\phi}_2} e^{(\hat{\phi}_0 + \tau_3 \hat{\phi}_3)/2}, \quad (\text{A8})$$

where now the matrix in the middle is unitary instead of Hermitian. Correspondingly, we change the parametrization of the bosonic valence block, A of Eq. (A2), from

$$\begin{aligned} A &= e^{(i\phi_0 + i\tau_3 \phi_3)/2} e^{i\tau_1 \phi_1 + i\tau_2 \phi_2} e^{(i\phi_0 + i\tau_3 \phi_3)/2} \\ &= e^{i\psi_1 + i\psi_2} \begin{pmatrix} \cos\theta e^{i\psi_1 - i\psi_2} & \sin\theta e^{i\rho} \\ -\sin\theta e^{-i\rho} & \cos\theta e^{-i(\psi_1 - i\psi_2)} \end{pmatrix}, \end{aligned} \quad (\text{A9})$$

in which in terms of the variables of Ref. [32]

$$\begin{aligned} \psi_1 + \psi_2 &= \phi_0, & \psi_1 - \psi_2 &= \phi_3, & \theta &= \sqrt{\phi_1^2 + \phi_2^2}, \\ \sin\rho &= \frac{\phi_1}{\theta}, & \cos\rho &= \frac{\phi_2}{\theta}, \end{aligned} \quad (\text{A10})$$

to

$$A_{\tau_3} = e^{(i\phi_0 + i\tau_3 \phi_3)/2} e^{\tau_1 \phi_1 + \tau_2 \phi_2} e^{(i\phi_0 + i\tau_3 \phi_3)/2}. \quad (\text{A11})$$

In other words, for those generators in which we change the fields from noncompact to compact in the ghost sector ($\hat{\phi}_{1,2}$), we change the fields from compact to noncompact in the quark sector (to be compared with the standard choice $\phi_2 = 0$ in Eq. (36)).

In this parametrization the measures for the matrices $w_{1,2}$ (parametrized by $\phi_{0,3}$ and $\hat{\phi}_{0,3}$) and the matrices w and \bar{w} (parametrized by $\phi_{1,2}$ and $\hat{\phi}_{1,2}$) of Ref. [32] factorize. Following section (3.1.2) of Ref. [32], our change in parametrization corresponds to an interchange of the variables Φ and θ , which leaves the measure (cf. Eq. (3.51) of Ref. [32]) invariant. We thus conclude that if the partition function for the two-flavor case is independent of the quark mass (as we showed it to be for the one-flavor case above), it is also independent of the quark mass for our new parametrization, if we follow the prescription given above.

¹⁷Note that the point $r = s = 0$ is singular.

¹⁸We denote the parameter ϕ of Ref. [32] by Φ here in order to avoid confusion.

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