On the consistency of the Aoki-phase

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Abstract

Lattice QCD with two flavors of Wilson fermions can exhibit spontaneous breaking of flavor and parity, with the resulting “Aoki phase” characterized by the non-zero expectation value $\langle \bar{\psi} \gamma_5 \tau_3 \psi \rangle \neq 0$. This phenomenon can be understood using the chiral effective theory appropriate to the Symanzik effective action. Within this standard analysis, the flavor-singlet pseudoscalar expectation value vanishes: $\langle i \bar{\psi} \gamma_5 \psi \rangle = 0$. A recent reanalysis has questioned this understanding, arguing that either the Aoki-phase is unphysical, or that there are additional phases in which $\langle i \bar{\psi} \gamma_5 \psi \rangle \neq 0$. The reanalysis uses the properties of probability distribution functions for observables built of fermion fields and expansions in terms of the eigenvalues of the hermitian Wilson-Dirac operator. Here I show that the standard understanding of the Aoki-phase can, in fact, be consistent with the approach used in the reanalysis. Furthermore, if one assumes that the standard understanding is correct, one can use the methods of the reanalysis to derive lattice generalizations of the continuum sum rules of Leutwyler and Smilga.
I. INTRODUCTION

New patterns of spontaneous symmetry breaking can arise in lattice theories away from the continuum limit. This paper concerns the example of lattice QCD (LQCD) with two flavors of (possibly improved) Wilson fermions. Aoki proposed long ago that the apparent masslessness of the pions at non-zero lattice spacing could be understood if there is a phase in which parity and flavor are spontaneously broken [1]. Numerical evidence for such a phase (largely in quenched studies) [2] was subsequently supported by theoretical analyses based on the linear sigma-model [3] and on applying chiral perturbation theory (χPT) to the continuum effective Lagrangian of Symanzik [4]. The latter analysis incorporates discretization errors in a systematic and theoretically well-established way, and uses the standard methods of continuum χPT. Near the continuum limit, it predicts two possible scenarios, depending on the sign of an unknown low-energy coefficient. In one scenario, flavor and parity are broken, and there is an Aoki-phase, while in the other (the “first-order” scenario) there is no spontaneous breaking of lattice symmetries. The present paper concerns the former scenario, and thus assumes that there are choices of gauge and fermion actions which lead to the appropriate sign of the low-energy coefficient.1

This analysis of the Aoki-phase has been recently questioned by Azcoiti, Di Carlo and Vaquero (ADV) [8], who study the pattern of spontaneous symmetry breaking (SSB) using probability distribution functions (p.d.f.s) of fermionic bilinears [9]. Given certain assumptions, they argue that either the pattern of non-vanishing condensates differs from that in the usual Aoki-phase (and that hermiticity is violated), or that there are phases additional to the Aoki-phase in which there is a differing pattern of condensates. Both possibilities are in contradiction with the standard χPT-based analysis. The χPT analysis (recapped below) predicts a non-zero value only for the condensate $\langle i\bar{\psi}\gamma_5\tau_3\psi \rangle$, and predicts only a single symmetry-breaking phase.

The main purpose of this paper is to point out a loophole in the assumptions made by ADV, one that allows the standard Aoki-phase to be present. There is no need for the presence of more exotic phases. Furthermore, if one assumes that the standard analysis is

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1 Recent unquenched simulations with unimproved twisted-mass fermions in fact indicate that the first-order scenario applies for both the Wilson gauge action [5] and the tree-level Symanzik improved gauge action [6], although an Aoki-phase is observed with the Wilson gauge action at stronger coupling [7].
correct, one can derive sum-rules for the eigenvalues of the hermitian Wilson-Dirac operator on the lattice, analogous to those derived by Leutwyler and Smilga in the continuum [10].

It will be useful to have in mind the main players in the following discussion. These are the zero-momentum parity and parity-flavor violating bilinears:

\[ C_0 = \frac{1}{N_{\text{site}}} \sum_n i\bar{\psi}\gamma_5\psi(n), \quad \text{and} \quad C_3 = \frac{1}{N_{\text{site}}} \sum_n i\bar{\psi}\gamma_5\tau_3\psi(n). \]  

(1.1)

Here \( n \) labels lattice sites, \( N_{\text{site}} \) is the number of such sites, and the fields are bare lattice flavor doublets. Note that \( C_0 \) and \( C_3 \) are dimensionless lattice quantities.

The remainder of this paper is organized as follows. The next section provides a brief summary of the \( \chi PT \) argument of Ref. [4], and gives some additional results for the “\( \epsilon \)-regime” that will be needed later. Section III then gives a brief summary of the p.d.f. method and the results relevant for its application to the Aoki-phase. An important point is that the results from the p.d.f. analysis are completely consistent with the predictions of \( \chi PT \), so that what is new about the approach of ADV is their use of eigenvalue decompositions. In Sec. IV I summarize the argument of ADV, pointing out its inconsistency with the \( \chi PT \) analysis. The core of this paper is Sec. V in which I explain the loophole in the argument of ADV, and give two examples of how this loophole might apply. I also present the above-mentioned sum-rules. I conclude with a summary and a brief discussion of generalizations in Sec. VI I include two appendices, the first describing the derivation of a result used in Sec. V, the second providing an alternative formulation of the sum-rules using microscopic spectral densities.

II. REVIEW OF \( \chi PT \) ANALYSIS OF AOKI-PHASE

In this section I recall the essential features of the analysis of Ref. [4]. Vacuum alignment for two flavors of Wilson fermions with no twisted mass term is determined at leading order in \( \chi PT \) by minimizing the potential\(^2\)

\[ V^\chi(\Sigma) = -\frac{c_1}{4} \text{Tr}(\Sigma + \Sigma^\dagger) + \frac{c_2}{16} \left[ \text{Tr}(\Sigma + \Sigma^\dagger) \right]^2. \]  

(2.1)

Here \( \Sigma \) is an \( SU(2) \) matrix proportional to the quark condensate, and the coefficients have magnitudes \( c_1 \sim m\Lambda^3_{\text{QCD}} \) and \( c_2 \sim a^2\Lambda^6_{\text{QCD}} \), with \( m \) the physical quark mass and \( a \) the lattice

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\(^2\) The analysis in this section is in an effective continuum theory, so that fields, masses etc. have their usual continuum dimensions.
To produce an Aoki-phase, the two terms in the potential must have comparable magnitudes, which occurs if $m \sim a^2 \Lambda_{\text{QCD}}^3$. This, together with $m \ll \Lambda_{\text{QCD}}$, is the power-counting used in this paper. Note that discretization errors linear in $a$ have been absorbed into the critical mass $m_c$.

The Aoki-phase scenario occurs when $c_2 > 0$. Recalling that $c_1$ is proportional to $m$ (with a positive coefficient of proportionality), one finds that for $|m|$ large enough that $|c_1| \geq 2c_2$, the condensate is aligned with $m$ just as in the continuum: $\Sigma_0 \equiv \langle \Sigma \rangle = \text{sign}(m) \mathbf{1}$. For smaller values of $|m|$, however, the potential is minimized by $\Sigma_0 = \exp(i\theta_0 \hat{n} \cdot \tau)$ with $\cos \theta_0 = c_1/(2c_2)$ and $\hat{n}$ a unit vector. The $SU(2)$ flavor symmetry $\Sigma \rightarrow U \Sigma U^\dagger$ is then broken to the $U(1)$ subgroup with $U = \exp(i\phi \hat{n} \cdot \tau)$. This results in two massless Goldstone pions, with the third pion having a mass proportional to $a$. The direction of the condensate can be fixed by adding a source term to the action, and the standard choice is to add the canonical twisted-mass term $\mu \bar{\psi} \gamma_5 \tau_3 \psi$, with $\psi$ the bare lattice $SU(2)$ doublet. This gives a mass to the (now pseudo-)Goldstone pions proportional to $\sqrt{\mu}$. One then sends the volume $V$ to infinity, followed by $\mu \rightarrow 0$, so that all pions are massive except in the final limit. This results in the condensate being aligned as $\Sigma_0 = \cos \theta_0 + i \sin \theta_0 \tau_3$, with the charged pions being massless and the neutral pion having $m_{\pi^0} \sim a\Lambda_{\text{QCD}}^2$.

An important point for the subsequent discussion is that taking $V \rightarrow \infty$ before $\mu \rightarrow 0$ implies that $m_{\pi^\pm} L \rightarrow \infty$, so that one is in the so-called “$p$-regime” for the charged pions. Were one to take the limits in the other order, i.e. $\mu \rightarrow 0$ and then $V \rightarrow \infty$, then the zero-momentum fluctuations in the charged pion directions would be unsuppressed, and one would be in the “$\epsilon$-regime” for these modes \[14\]. I will distinguish between expectation values obtained in these two orders of limits using the subscripts “$p$” and “$\epsilon$”. While this has the advantage of linking the limits to familiar names, one should also keep in mind that both $p$- and $\epsilon$-regimes are defined more generally. In particular, they are defined also for finite $V$—as the regimes in which $m_{\pi} L \gg 1$ or $\ll 1$, respectively, with $L$ the box size. I am not making use of the full extent of these regimes, but rather only the single points in each regime reached in the limits described above. Note that $m_{\pi^0} L \sim aL \rightarrow \infty$ in both regimes.

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3 More explicitly, in terms of the low-energy coefficients in the chiral Lagrangian, $c_1 = 2f^2 B_0 m$ and $c_2 = -16W'W_0^2 a^2$, where I use the notation of Ref. \[11\]. The physical quark mass is $m = Z_m (m_0 - m_c)/a$, with $m_0$ the bare Wilson quark mass and $m_c$ the critical mass.

4 This analysis of course receives corrections from higher order terms in $\chi$PT, as described in Refs. \[12, 13\].
since $a$ is held fixed, so that fluctuations in the neutral pion direction are always suppressed. This means that both regimes for the lattice theory differ from the corresponding regimes in the continuum. For example, the continuum $\epsilon$-regime has unsuppressed zero-momentum modes in all three pion directions.

Using the leading order relations between quark bilinears and $\Sigma$, it follows that, in the Aoki-phase, the parity and flavor-breaking condensates are

$$\frac{Z_P}{a^3} \langle C_3 \rangle_p = i (f^2 B_0/2) \text{Tr} \left( \tau_3 \left[ \Sigma_0 - \Sigma_0^\dagger \right] \right) = - \sin \theta_0 2 f^2 B_0 , \quad (2.2)$$

$$\frac{Z_{P_0}}{a^3} \langle C_0 \rangle_p = (f^2 B_0/2) i \text{Tr} \left( \Sigma_0 - \Sigma_0^\dagger \right) = 0 . \quad (2.3)$$

The matching factors and powers of $a$ are needed to convert from lattice to continuum normalization. Here $f$ and $B_0$ are the standard low-energy coefficients of $\chi$PT, in terms of which the continuum condensate with a standard mass term is

$$\langle \bar{\psi} \psi \rangle_{\text{cont}} = \langle \bar{u} u + \bar{d} d \rangle_{\text{cont}} = - \text{sign}(m) 2 f^2 B_0 . \quad (2.4)$$

On the lattice, only the pseudoscalar condensates can be determined, due to the mixing of $\bar{\psi} \psi$ with the identity operator. Thus it is the results of Eqs. (2.2) and (2.3) that are pertinent. I emphasize two features of these results: (i) The magnitude of the flavor-non-singlet condensate varies as one moves across the Aoki-phase, with the maximum at $m = c_1 = 0$ being equal to $|\langle \bar{\psi} \psi \rangle_{\text{cont}}|$ when appropriately normalized; (ii) The vanishing of the flavor-singlet pseudoscalar condensate is true for any $\Sigma_0 \in SU(2)$, and is not special to the particular vacuum of the Aoki-phase.

This completes the discussion of the analysis of Ref. [4]. For the following, it will be necessary to generalize the results in two ways. The first is to determine the zero-momentum two-point functions of the bilinears in the $p$-regime. The results are simple (and can be written in a way that avoids $Z$-factors):

$$\langle C_3^2 \rangle_p = \langle C_3 \rangle_p^2 , \quad (2.5)$$

$$\langle C_0^2 \rangle_p = \langle C_0 \rangle_p^2 = 0 . \quad (2.6)$$

In words, only the disconnected contributions remain when $N_{\text{site}} \to \infty$. This is because, in the $p$-regime, the connected parts receive contributions from massive intermediate states, and thus are localized in space. Although one of the $1/N_{\text{site}}$ factors is canceled by translations, the other remains and causes the contributions to vanish when $N_{\text{site}} \to \infty$. 
The second generalization is to the $\epsilon$-regime. As discussed above, zero-momentum fluctuations of $\Sigma$ in the charged-pion directions are unsuppressed, and one must integrate the zero-modes over the Goldstone manifold \([14]\). Non-zero-momentum modes can be ignored at leading order. The result is that the flavor-parity breaking condensate now vanishes

$$
\langle C_3 \rangle_\epsilon = \frac{a^3}{Z_P} \int_{\Sigma_0 \in SU(2)/U(1)} i(f^2 B_0/2) \text{Tr} \left( \tau_3 \left[ \Sigma_0 - \Sigma_0^\dagger \right] \right) = 0.
$$

(2.7)

By contrast, the average of the square of the zero-momentum mode does not vanish:

$$
\langle C_3^2 \rangle_\epsilon = \left( \frac{a^3}{Z_P} \right)^2 \int_{\Sigma_0 \in SU(2)/U(1)} (i f^2 B_0/2)^2 \left\{ \text{Tr} \left( \tau_3 \left[ \Sigma_0 - \Sigma_0^\dagger \right] \right) \right\}^2
\]

$$
= \frac{1}{3} \left( \frac{a^3}{Z_P} \right)^2 (\sin \theta_0 f^2 B_0)^2
$$

(2.8)

Comparing the final expression to Eq. (2.5) one sees how averaging over the Goldstone manifold reduces the size of the squared condensate by the geometrical factor of $1/3$. For the flavor-singlet pseudoscalar, however, the corresponding expectation values vanish,

$$
\langle C_0 \rangle_\epsilon = \langle C_0^2 \rangle_\epsilon = 0,
$$

(2.10)

because the vacuum manifold is simply the origin.

It is straightforward to extend these results to higher powers of the $C_a$, with results that are quoted and used in Appendix B.

### III. PROBABILITY DENSITY FUNCTIONS FOR FERMION BILINEARS

The ADV analysis of SSB for Wilson fermions uses probability distribution functions for fermion bilinears. Here I briefly recall the essential properties of these p.d.f.s. The p.d.f. is familiar for scalar field theories, where it is defined by inserting $\delta(C - \frac{1}{N_{\text{site}}} \sum_n \phi_n)$ in the functional integral (considering here a real scalar field). It is related to the constraint effective potential, $P(C) = \exp[-N_{\text{site}} \mathcal{V}_{\text{constr.}}(C)]$ and is a useful tool for studying symmetry breaking. In particular, in the absence of source terms, it is invariant under the symmetries of the action. For example, if there is a $\phi \rightarrow -\phi$ symmetry, and this is spontaneously broken, then $P(C) = (1/2)[\delta(C - C_0) + \delta(C + C_0)]$ when $N_{\text{site}} \rightarrow \infty$, with $C_0$ the magnitude of the
expectation value in the presence of an infinitesimal source. If the symmetry is unbroken, then \( P(C) = \delta(C) \).

The construction of a p.d.f. is generalized to fermion bilinears in Ref. [9]. It is a non-trivial result that the resulting p.d.f. can be used in the same way as for scalar field theories, and, in particular, as a tool to study SSB. In the present instance the p.d.f.s of interest are those for \( C_0 \) and \( C_3 \). If one could calculate \( P(C_0) \) and \( P(C_3) \) using the method of Ref. [9] then one could deduce whether SSB occurs and the nature of any broken phases.

ADV make particular use of \( P(C_0) \) and \( P(C_3) \) in the “Gibbs state”, which means here that one evaluates them with no twisted-mass source term, but takes the \( N_{\text{site}} \to \infty \) limit. As noted in the previous section, this puts the theory in the \( \epsilon \)-regime, in which symmetries are manifest. Thus the expectation values of \( C_a, a = 0, 3 \) vanish, because of parity and flavor-parity respectively:

\[
\langle C_a \rangle_\epsilon \equiv \lim_{N_{\text{site}} \to \infty} \int dC_a \ P(C_a) \ C_a = 0.
\]  

(3.1)

Note that this result gives no information about SSB, since it holds irrespective of whether the symmetries would spontaneously break were the limits taken in the other order (\( N_{\text{site}} \to \infty \) followed by the twisted-mass source term vanishing). It is also possible, as suggested by ADV, that there are several vacua, each with differing patterns of condensates, which are averaged over in the Gibbs state. leading to a vanishing result.

Higher moments of the p.d.f.s are, however, order parameters for SSB. Following ADV, I focus mostly on the second moment, for which one expects [8, 9]

\[
\langle C_a^2 \rangle_\epsilon = \lim_{N_{\text{site}} \to \infty} \int dC_a \ P(C_a) \ C_a^2 = f_{\text{geom}} \times |\langle C_a \rangle_p|^2.
\]  

(3.2)

Here \( f_{\text{geom}} \) is a non-vanishing geometrical factor which depends on the vacuum manifold. It follows from (3.2) that, if there is no SSB, and \( \langle C_a \rangle_p = 0 \), then \( \langle C_a^2 \rangle_\epsilon \) will vanish. On the other hand, if there is SSB and \( \langle C_a \rangle_p \neq 0 \), then \( \langle C_a^2 \rangle_\epsilon \) will be non-vanishing.

The value of \( f_{\text{geom}} \) can be determined if the vacuum manifold is known. For a single vacuum, \( f_{\text{geom}} = 1 \), while for the continuous \( U(1) \) (complex scalar field), \( SU(2)/U(1) \) (Aoki-phase) and \( SU(2) \) (continuum chiral symmetry breaking) manifolds the factor is \( f_{\text{geom}} = 1/2, 1/3 \) and \( 1/4 \), respectively. These are simply obtained by averaging the squared projection of the field onto a fixed axis over the respective manifolds. More complicated vacuum manifolds with disconnected components would lead to other, less simple, values of \( f_{\text{geom}} \).
ADV apply this methodology to the Aoki-phase. If the standard analysis holds, then
\(<C_0>_p = 0\) while \(<C_3>_p \neq 0\), and one then finds
\[
\langle C_3^2 \rangle_\epsilon = \frac{|\langle C_3_>_p|^2}{3} \neq 0 \tag{3.3}
\]
\[
\langle C_0^2 \rangle_\epsilon = 0 \tag{3.4}
\]
The issue in the following is whether these results are correct, and in particular, whether they are consistent with expressions in terms of eigenvalues of the hermitian Wilson-Dirac operator. If not, the standard understanding of the Aoki-phase must be wrong. This holds also for the extension of the above results to higher powers of the \(C_a\), which are straightforward to derive, and which are quoted and used in Appendix B.

I close this section by noting that the results of the p.d.f. analysis can also be obtained using \(\chi PT\). This is shown by the consistency of Eqs. (2.9) and (2.10) from the previous section with Eqs. (3.3) and (3.4). This consistency is, in fact, preordained, because the required average over the vacuum manifold is identical in the two approaches. Each approach has its strengths and weaknesses: \(\chi PT\) adds the specific prediction for \(\langle C_3_>_p\), Eq. (2.2), while the p.d.f. analysis does not require an expansion in \(m\) and \(a\). Still, for small \(m \sim a^2 \Lambda^3_{QCD}\), as considered here, one does not need the p.d.f. methodology to pose the puzzle noted by ADV.

IV. THE ARGUMENT OF ADV

ADV base their argument on the expressions for the expectation values in terms of the (real dimensionless) eigenvalues of the hermitian Wilson-Dirac operator, \(H_W = \gamma_5 D_W\). Denoting these eigenvalues by \(\lambda_j\), and including a bare lattice twisted mass, \(\mu_0\), one has
\[
\langle C_0 \rangle = \frac{2i}{N_{\text{site}}} \left\langle \sum_j \frac{\lambda_j}{\mu_0^2 + \lambda_j^2} \right\rangle \overset{\mu_0 \to 0}{\longrightarrow} \frac{2i}{N_{\text{site}}} \left\langle \sum_j \frac{1}{\lambda_j} \right\rangle \tag{4.1}
\]
\[
\langle C_3 \rangle = -\frac{2}{N_{\text{site}}} \left\langle \sum_j \frac{\mu_0}{\mu_0^2 + \lambda_j^2} \right\rangle \overset{\mu_0 \to 0}{\longrightarrow} 0 \tag{4.2}
\]
\[
\langle C_a^2 \rangle = \langle C_a^2 \rangle_{\text{disc}} + \langle C_a^2 \rangle_{\text{conn}} \tag{4.3}
\]
\[
\langle C_0^2 \rangle_{\text{disc}} = -\frac{4}{N_{\text{site}}^2} \left\langle \left( \sum_j \frac{\lambda_j}{\lambda_j^2 + \mu_0^2} \right)^2 \right\rangle \overset{\mu_0 \to 0}{\longrightarrow} -\frac{4}{N_{\text{site}}^2} \left\langle \left( \sum_j \frac{1}{\lambda_j} \right)^2 \right\rangle \tag{4.4}
\]
\[
\langle C_0^2 \rangle_{\text{conn}} = \langle C_3^2 \rangle_{\text{conn}} = \frac{2}{N_{\text{site}}} \left\langle \sum_j \frac{\lambda_j^2 - \mu_0^2}{(\lambda_j^2 + \mu_0^2)^2} \right\rangle \overset{\mu_0 \to 0}{\longrightarrow} \frac{2}{N_{\text{site}}} \left\langle \sum_j \frac{1}{\lambda_j^2} \right\rangle \tag{4.5}
\]
\[
\langle C^2_3 \rangle_{\text{disc}} = \frac{4}{N_{\text{site}}} \left( \sum_j \frac{\mu_0}{\lambda_j^2 + \mu_0^2} \right)^2 \xrightarrow{\mu_0 \to 0} 0
\]  

(4.6)

The first result on each line can be used to obtain the “p-regime” expectation values (i.e. \(N_{\text{site}} \to \infty\) and then \(\mu_0 \to 0\)). Taking the limits in this order means that the spectrum of eigenvalues becomes continuous. The second result on each line (i.e. that with \(\mu_0 = 0\)) gives, once \(N_{\text{site}} \to \infty\), the “\(\epsilon\)-regime” expectation values.

Consider first the linear moments, Eqs. (4.1) and (4.2). Applying a parity transformation flips the sign of \(\lambda\) and \(\mu_0\), and thus averaging over a configuration and its parity conjugate leads to a vanishing \(\langle C_0 \rangle\) in both p- and \(\epsilon\)-regimes.\(^5\) This is consistent with the standard expectations, Eqs. (2.3) and (3.1). The prediction of (4.2) that \(\langle C^3_3 \rangle_{\epsilon} = 0\) is also consistent with Eq. (3.1). In the p-regime, however, one can obtain a non-vanishing expectation

\[
\langle C^3_3 \rangle_p = -\lim_{\mu_0 \to 0} \lim_{N_{\text{site}} \to \infty} \frac{2}{N_{\text{site}}} \left( \sum_j \frac{\mu_0}{\mu_0^2 + \lambda_j^2} \right) = -2\pi \langle \rho_U(0) \rangle_p \equiv -2\pi \rho(0) .
\]  

(4.7)

This is the standard Banks-Casher relation applied to the present context, in which \(\rho_U(\lambda)\) is the eigenvalue density of \(H_W\) per unit (dimensionless) volume on a given configuration (which can be defined when \(N_{\text{site}} \to \infty\)) and \(\rho(\lambda)\) is its average over configurations. For the Aoki-phase scenario to hold one must have \(\rho(0) \neq 0\), and to match with the \(\chi\)PT prediction (2.2) requires

\[
\rho(0) = \frac{a^3 \sin \theta_0 f^2 B_0}{Z_P} .
\]  

(4.8)

Thus far the results are conventional and uncontroversial.

The apparent problems with the Aoki-phase concern the expectation value \(\langle C^2_0 \rangle\). In the standard scenario, this is expected to vanish in both the \(\epsilon\)-regime [Eqs. (2.10) and (3.4)] and p-regime [Eq. (2.6)]. The expressions in terms of eigenvalues—Eqs. (4.3–4.5)—do not, however, vanish under parity averaging, reflecting the fact that \(C^2_0\) is even under parity. The issue is whether they vanish when \(N_{\text{site}} \to \infty\).

ADV argue that, assuming the standard properties of \(C^2_3\) in the Aoki-phase, \(\langle C^2_0 \rangle\) does not vanish, in contradiction to the standard Aoki-phase scenario. They reach this conclusion by considering the two possibilities for the behavior of the eigenvalues under parity:

\(^5\) At \(a \neq 0\) one does not have an index theorem and the corresponding zero-modes related to topology. There can be isolated zero-modes on some configurations, as discussed further in the next section, but these will introduce an additional suppression of \(\mu_0^2\) from the fermion determinant, and thus do not contribute when \(\mu_0 \to 0\) to either of the linear moments. This holds also for the quadratic moments.
1. \( \rho_U(\lambda) = \rho_U(-\lambda) \): the eigenvalue distribution for \( \mu_0 = 0 \) becomes even in \( \lambda \) on each configuration when \( N_{\text{site}} \to \infty \). This is what happens if averaging over an infinite volume effectively includes a parity average, which is what one would expect. In this case \( \langle C_0^2 \rangle_{\text{disc}} \) vanishes in both regimes since the summand in (4.4) is odd in \( \lambda \). ADV focus (in their section IV) on the \( \epsilon \)-regime. Since \( \langle C_3^2 \rangle_{\text{disc}, \epsilon} \) vanishes identically [see eq. (4.6)], it follows that

\[
\langle C_0^2 \rangle_{\epsilon} = \langle C_0^2 \rangle_{\text{conn}, \epsilon} = \langle C_3^2 \rangle_{\text{conn}, \epsilon} = \langle C_3^2 \rangle_{\epsilon}.
\] (4.9)

Thus if \( \langle C_3^2 \rangle_{\epsilon} \) is non-vanishing, then so is \( \langle C_0^2 \rangle_{\epsilon} \). This is in manifest contradiction with Eqs. (2.9) and (2.10) [or equivalently with Eqs. (3.3) and (3.4)], and the standard picture of the Aoki-phase fails. To obtain consistency with (4.9) ADV postulate the presence of an additional phase with non-vanishing \( \langle C_0 \rangle_p \).

2. \( \rho_U(\lambda) \neq \rho_U(-\lambda) \): the eigenvalue distribution is not symmetric on a given configuration, even in the \( N_{\text{site}} \to \infty \) limit. In this part of the argument (section III of their paper) ADV keep \( \mu_0 \) non-zero (they call it \( m_t \)) while sending \( N_{\text{site}} \to \infty \), and thus they are working in the \( p \)-regime.\(^6\) Since there are then no exactly massless particles, it follows, as discussed above, that connected two-point functions vanish when \( N_{\text{site}} \to \infty \). ADV conclude that

\[
\langle C_0^2 \rangle_p = \lim_{N_{\text{site}} \to \infty} \langle C_0^2 \rangle_{\text{disc}} = -4 \left\langle \int d\lambda \frac{\rho_U(\lambda)}{\lambda} \right\rangle^2,
\] (4.10)

which, by assumption, is negative definite. This is in contradiction with the vanishing result (2.6) expected in the Aoki-phase.\(^7\)

Having considered both symmetric and asymmetric \( \rho_U(\lambda) \), and finding both in contradiction with the Aoki-phase, ADV conclude that the standard Aoki-phase scenario must be incomplete.

I emphasize that, if the argument of ADV is correct, then one must conclude that the standard \( \chi \)PT-based analysis is incorrect. For small enough \( m \) and \( a^2 \), the \( \chi \)PT analysis

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\(^6\) In general, \( \rho_U(\lambda) \) depends on \( \mu_0 \). Here, however, \( \mu_0 \) is infinitesimal, so the flip in sign of \( \mu_0 \) under parity does not affect \( \rho_U(\lambda) \).

\(^7\) ADV expand further on the implications of \( \langle C_0^2 \rangle_p < 0 \), which violates hermiticity in the continuum limit. For my purposes it is, however, sufficient to show that the result (4.10) is in contradiction with the Aoki-phase expectations.
unambiguously predicts only one possible pattern of symmetry breaking, in which $\langle C_0^2 \rangle_p = \langle C_0^2 \rangle_\epsilon = 0$. This is simply in contradiction with both of the possibilities enumerated above, and in particular with Eqs. (4.9) and (4.10).

V. CONSISTENCY OF THE AOKI-PHASE WITH EIGENVALUE SUMS

The conclusion of ADV’s argument is surprising. One would not expect that the Aoki-phase scenario, based as it is on a straightforward application of the methods of effective field theory, could be invalidated by simple properties of eigenvalues of $H_W$, especially since these properties do not appear to be in conflict with the assumptions of the $\chi$PT analysis.

In fact, there is a loophole in the argument of ADV. This arises because the summand in Eq. (4.4) is infrared divergent in the $\epsilon$-regime. This allows an asymmetry in the spectrum which is subleading as $N_{\text{site}} \to \infty$, and which does not contribute in the infrared regulated $p$-regime, to nevertheless contribute to $\epsilon$-regime expressions. In this way it is possible for $\langle C_0^2 \rangle_{\text{disc},p} = 0$ while $\langle C_0^2 \rangle_{\text{disc},\epsilon} \neq 0$. Disconnected and connected contributions to $\langle C_0^2 \rangle_\epsilon$, which have opposite signs, can then cancel, leading to the desired result $\langle C_0^2 \rangle_\epsilon = 0$.

I stress that showing this possibility exists simply demonstrates that one cannot make a judgment about the Aoki-phase scenario using the basic properties of the eigenvalues of $H_W$. The Aoki-phase is an allowed option. To determine whether it actually occurs, however, requires further input, such as that provided by applying $\chi$PT to the Symanzik effective Lagrangian. Using this input, which predicts the Aoki-phase (assuming $c_2 > 0$), one can turn the ADV argument around and deduce sum-rules that the eigenvalues must satisfy. These are analogues of the Leutwyler-Smilga sum-rules for continuum QCD \cite{10}.

That the expectation values $\langle C_0^2 \rangle_{\text{disc},p}$ and $\langle C_0^2 \rangle_{\text{disc},\epsilon}$ can differ is an example of the non-commutativity of the $\mu_0 \to 0$ and $N_{\text{site}} \to \infty$ limits. This non-commutativity is familiar from the properties of $\langle C_3 \rangle$ noted above [see Eq. (4.7) and preceding discussion]. Another example is the behavior of $\langle C_0^2 \rangle_{\text{conn}} = \langle C_3^2 \rangle_{\text{conn}}$, and it will be useful to describe this as a warm-up exercise before explaining the loophole.

In the $p$-regime one expects $\langle C_0^2 \rangle_{\text{conn}}$ to vanish because only massive intermediate states contribute. To see how this works with eigenvalues, one writes

$$
\langle C_0^2 \rangle_{\text{conn},p} = \lim_{\mu_0 \to 0} \lim_{N_{\text{site}} \to \infty} \frac{2}{N_{\text{site}}} \int d\lambda \frac{\lambda^2 - \mu_0^2}{(\lambda^2 + \mu_0^2)^2} \rho(\lambda).
$$

(5.1)
Here I have used the result that averaging over configurations allows one to define a continuous density \( \rho(\lambda) \) prior to taking \( N\text{site} \to \infty \), and I am assuming that \( 1/N\text{site} \) and \( \mu_0 \) are small enough that \( \rho(\lambda) \) does not depend on them. The key point is that the integral on the right-hand-side is finite, so that \( \langle C_0^2 \rangle_{\text{conn},p} \to 0 \) when \( N\text{site} \to \infty \) due to the overall factor of \( 1/N\text{site} \). The only possible sources of divergence in the integral are the infrared and ultraviolet regions. Only the first two terms in the Taylor expansion of \( \rho \) about \( \lambda = 0 \) can lead to infrared divergences, but their contributions vanish for any non-zero \( \mu_0 \). The ultraviolet divergence (arising because \( \rho \propto \lambda^3 \) for \( \lambda \gg a\Lambda_{\text{QCD}} \)) is regulated on the lattice because there is cut-off on eigenvalues, \( \lambda_{\text{max}} \approx 1.8 \).

By contrast, in the \( \epsilon \)-regime, \( \langle C_0^2 \rangle_{\text{conn}} \) has the infrared-divergent summand \( 1/(N\text{site}\lambda_j)^2 \). Since \( \rho(0) \neq 0 \), the low eigenvalues are approximately uniformly distributed with spacing \( \Delta\lambda \sim 1/[N\text{site} \rho(0)] \) and with \( \lambda_{\text{min}} \sim 1/[N\text{site} \rho(0)] \). They thus give a non-vanishing contribution to \( \langle C_0^2 \rangle_{\text{conn}} \) when \( N\text{site} \to \infty \) [one that cannot be represented as an integral over \( \rho(\lambda) \)]. This is qualitatively consistent with the expectation \( (3.3) \) from the p.d.f. analysis. To agree quantitatively with the \( \chi \)PT result \( (2.9) \) requires that the following sum-rule hold:

\[
\lim_{N\text{site} \to \infty} \frac{2}{N\text{site}^2} \left( \sum_j \frac{1}{\lambda_j^2} \right) = \frac{4\pi^2}{3} \rho(0)^2 = \frac{4}{3} \left( \frac{a^3}{ZP} \sin \theta_0 f^2 B_0 \right)^2 . \tag{5.2}
\]

This constrains the distribution of the small eigenvalues of \( H_W \). Note that it must hold separately for each value of \( m \) throughout the Aoki-phase.

With this warm-up completed I now return to main quantity of interest, \( \langle C_0^2 \rangle_{\text{disc}} \). For the Aoki-phase to be consistent this quantity must vanish in the \( p \)-regime and cancel \( \langle C_0^2 \rangle_{\text{conn}} \) in the \( \epsilon \)-regime. Vanishing in the \( p \)-regime requires

\[
\langle C_0^2 \rangle_{\text{disc},p} = - \lim_{\mu_0 \to 0} \left\langle \left( \int d\lambda \frac{\lambda [\rho_U(\lambda) - \rho_U(-\lambda)]}{\lambda^2 + \mu_0^2} \right)^2 \right\rangle = 0 . \tag{5.3}
\]

Since the integrand is finite in the infrared for any non-zero \( \mu_0 \), this relation is satisfied if the density is symmetric:

\[
\delta \rho_U(\lambda) \equiv \rho_U(\lambda) - \rho_U(-\lambda) = 0 . \tag{5.4}
\]

I stress that the condition \( (5.4) \) concerns only the spectrum in the \( N\text{site} \to \infty \) limit—indeed, it is only in this limit that \( \rho_U \) (and thus \( \delta \rho_U \)) becomes well-defined.

---

\( ^8 \) That the ultraviolet divergence is subleading in \( 1/N\text{site} \) is as in the continuum, as has been discussed in Ref. [10]. This result applies also for the other eigenvalue sums considered below.
The question then is how $\langle C^2_0 \rangle_{\text{conn}, \epsilon}$ can be non-zero and cancel with $\langle C^2_0 \rangle_{\text{disc}, \epsilon}$, i.e. how the sequence of equalities in Eq. (4.9) of ADV’s first possibility can fail. From Eqs. (4.4), (4.5) and (5.2) the requirement is that

$$\lim_{N_{\text{site}} \to \infty} \frac{1}{N_{\text{site}}^2} \left\langle \left( \sum_j \frac{1}{\lambda_j} \right)^2 \right\rangle = \frac{\pi^2}{3} \rho(0)^2,$$

(5.5)

This relation must hold throughout the Aoki-phase (and, in fact, outside this phase too, where $\rho(0)$ vanishes). The issue is whether the left-hand-side can be non-vanishing given the symmetry property (5.4). This is possible if there is an asymmetry which, while vanishing when $N_{\text{site}} \to \infty$, is enhanced by the infrared divergence in the summand so that $\sum_j 1/(N_{\text{site}}\lambda_j)$ does not become $\int d\lambda \rho_U(\lambda)/\lambda$ when $N_{\text{site}} \to \infty$. If it did have this limit then the resulting integral would vanish given the symmetry of $\rho_U(\lambda)$ and one would be back to the first inconsistency noted by ADV.9

To show that it is possible for the sum-rule (5.5) to be satisfied I need to recall the properties of the spectrum of $H_W$. There is a wealth of literature on this topic, and I will use particularly the results and insights from Refs. [15, 16, 17, 18, 19, 20]. As noted above, exact zero-modes of $H_W$ are suppressed by its determinant and are not relevant. What is important is that the spectrum is known to be asymmetric on almost all configurations. This asymmetry is a remnant of the exact zero-modes of the Dirac operator which are present in the continuum limit on topologically non-trivial configurations. On the lattice these would-be exact zero modes end up as near-zero modes of $H_W$ and lead to an asymmetry, as described in more detail in Appendix A. I expect that the typical magnitude of the resulting asymmetry (defined on a given configuration as the difference between the number of modes with $\lambda_j > 0$ and $\lambda_j < 0$) depends on $a$ and the lattice volume $V = a^4 N_{\text{site}}$ as

$$|n_{\text{asym}}| \sim a \sqrt{V} \Lambda^3_{\text{QCD}}.$$

(5.6)

There are several arguments which support this parametric dependence. The most simple is to note that, in the continuum, the typical number of zero modes scales as $|n_{\text{zero}}| \sim \sqrt{mV\rho_D(0)}$, with $\rho_D(0) \sim \Lambda^3_{\text{QCD}}$ the eigenvalue density (per unit volume) of the Dirac operator [10]. This result is for the $p$-regime, which is appropriate since the neutral pion is in its $p$-regime on the lattice. Now, in the Aoki-phase, symmetry breaking by mass

9 The limit in Eq. (4.5) gives the principal part, which vanishes if $\rho_U$ is symmetric.
terms competes with that from $O(a^2)$ discretization effects, the latter being dominant in the center of the phase. Thus it is plausible that one can use the continuum formula with the replacements $m \rightarrow a^2 \Lambda_{\text{QCD}}^3$ and $n_{\text{zero}} \rightarrow n_{\text{asym}}$, leading to Eq. (5.6). Further arguments in support of this relation are given in Appendix A.

Another result needed below is that would-be exact zero-modes are expected to have eigenvalues shifted to $\lambda \sim (a \Lambda_{\text{QCD}})^q$ by discretization effects. Here $q$ is an unknown power that I argue below may be $q = 3$.

The result (5.6) for the spectral asymmetry is consistent with the $p$-regime requirement (5.4), because one must divide by $N_{\text{site}}$ to obtain the spectral density:

$$\int d\lambda \delta \rho_U(\lambda) = \lim_{N_{\text{site}} \to \infty} \frac{n_{\text{asym}}}{N_{\text{site}}} = 0.$$  (5.7)

To satisfy the $\epsilon$-regime requirement (5.5) requires consideration of how the asymmetry depends on $\lambda$. For illustration assume that there are more positive than negative eigenvalues on a particular configuration. Due to eigenvalue repulsion, one expects that the extra eigenvalues will impact the spectrum over the region $0 < \lambda < (a \Lambda_{\text{QCD}})^q$. To satisfy (5.5) this impact must be appropriately peaked at small $\lambda$. I give two examples of how this could work.

- The first is simple: I assume that the spectral asymmetry manifests itself by the presence of $O(1)$ extra small (positive) eigenvalues with $\lambda_j \sim 1/[N_{\text{site}} \rho(0)]$, while the remaining eigenvalues giving rise to the asymmetry are distributed in such a way as to give a contribution to $\sum_j 1/(N_{\text{site}} \lambda_j)$ which vanishes when $N_{\text{site}} \to \infty$. As shown by the second example, this requires the asymmetry to be less peaked than a $1/\sqrt{\lambda}$ singularity.

With these assumptions, $\sum_j 1/(N_{\text{site}} \lambda_j) \sim \rho(0)$, and so the square of this sum gives $\langle C_{\theta}^2 \rangle_{\text{disc}, \epsilon} \sim \rho(0)^2$. This has the correct magnitude to allow the sum-rule (5.5) to be satisfied.

Note that in this example I am not making particular use of the dependence (5.6) of the asymmetry on $a$ and $V$ (nor of the arguments given in Appendix A). It is, however, somewhat artificial to assume an $O(1)$ delta-function-like contribution to the asymmetry.

- In the second example, the asymmetry is spread continuously over the range $0 < \lambda < \frac{1}{4}$.
For finite $N_{\text{site}}$, the discrete sum over eigenvalues can be approximated by an integral aside from end effects which can be accounted for choosing the limits of integration appropriately. In this sense, one can consider $\delta \rho_U(\lambda)$ for finite $N_{\text{site}}$. The behavior I assume is

$$\delta \rho_U(\lambda) \sim \frac{(a \Lambda_{\text{QCD}})^{3-q/2}}{\sqrt{\lambda N_{\text{site}}}}, \quad (5.8)$$

in which the key feature is the $1/\sqrt{\lambda}$ singularity. The other factors are chosen so that one obtains the desired spectral asymmetry:

$$n_{\text{asym}} = N_{\text{site}} \int_0^{(a \Lambda_{\text{QCD}})^q} d\lambda \delta \rho_U(\lambda) \sim (a \Lambda_{\text{QCD}})^3 \sqrt{N_{\text{site}}} \sim a \sqrt{V} \Lambda_{\text{QCD}}^3. \quad (5.9)$$

The sum in (5.5) can then be approximated by an integral with the lower limit regulated with a quantity of order $\lambda_{\text{min}} \sim 1/[N_{\text{site}} \rho(0)]$:

$$\sum_j \frac{1}{N_{\text{site}} \lambda_j} \approx \int_{1/[N_{\text{site}} \rho(0)]}^{(a \Lambda_{\text{QCD}})^q} d\lambda \frac{\delta \rho_U(\lambda)}{\lambda} \sim (a \Lambda_{\text{QCD}})^{3-q/2} \rho(0)^{1/2} \sim (a \Lambda_{\text{QCD}})^{(9-q)/2}. \quad (5.10)$$

Here I have used $\rho(0) \sim (a \Lambda_{\text{QCD}})^3$ from Eq. (4.8). The key point is that the result (5.10) has a non-zero (and non-infinite) limit as $N_{\text{site}} \to \infty$. Inserting (5.10) into Eq. (5.5) then leads to a non-zero result for $\langle C^{(2)}_0 \rangle_{\text{disc}, \epsilon}$.

In addition, recalling that $\rho(0) \propto (a \Lambda_{\text{QCD}})^3$, one sees that for the $a$ dependence on both sides of Eq. (5.5) to match requires $q = 3$.

While this example is perhaps more realistic than the first, I stress that it only works if $\delta \rho$ diverges as $1/\sqrt{\lambda}$ and not for other powers.

I do not know if either of these examples represents the actual behavior. Presumably it should be possible to determine more detailed information on the distributions of low eigenvalues, as has been done in the continuum limit using the methods of random matrix theory. A small step in this direction has been taken in Ref. [21].

The description of the loophole given above is somewhat awkward and unsystematic. This shortcoming can be addressed in part by formulating the required consistency conditions in terms of the microscopic spectral density and correlations. This is done in Appendix B. Also included in this appendix is some discussion of how the consistency conditions extend to higher orders (corresponding to sum-rules with higher overall powers of $\lambda^{-1}$).
VI. CONCLUSIONS

The major aim of this paper has been to show the Aoki-phase scenario is not ruled out by the arguments of ADV. The examples presented in the previous section demonstrate this—the set of possibilities considered by ADV is incomplete. The “survival” of the Aoki-phase is consistent with the intuition that one cannot rule out the results of $\chi$PT using only general properties of eigenvalues of $H_W$.

If one accepts the standard analysis of the Aoki-phase, then one finds non-trivial conditions that must be obeyed by the eigenvalues of the hermitian Wilson-Dirac operators. These are the sum-rules (5.2) and (5.3), which can also be formulated as constraints on integrals of microscopic spectral correlators [Eqs. (B8) and (B9) respectively]. There are, in fact, an infinite set of these sum-rules, involving products of any even number of inverse-eigenvalues. While at first sight it may seem daunting that the eigenvalues of $H_W$ must be distributed so as to satisfy all these sum-rules, I show in Appendix B how each sum-rule constrains an essentially independent eigenvalue correlation function, making it more plausible that they can all be satisfied. The need to satisfy an infinite set of sum-rules is not special to the lattice theory. Indeed, for actions with chiral symmetry (as in the continuum analysis of Leutwyler and Smilga), the eigenvalues of the Dirac operator in each topological charge sector must satisfy an analogous infinite set of sum-rules. In this case, the sum-rules can be solved, and there is a large body of work successfully comparing the solutions to numerical results from overlap and related fermions (see, for example, the review in Ref. [22]). It would be of considerable interest if the solutions could be extended to the sum-rules discussed here.

One might wonder what can be learned about the other scenario predicted by $\chi$PT—that involving a first-order transition. The answer appears to be very little. In this case $\rho(\lambda)$ always has a gap, there is no SSB, there are no massless Goldstone pions, and thus no $\epsilon$-regime. One expects from $\chi$PT or from the p.d.f. analysis that $\langle C_a \rangle = \langle C_2^a \rangle = 0$ for both $a = 0, 3$. The consistency of these results with the expressions in terms of eigenvalues is almost trivial, because with a gap there are no infrared divergences.

One might also wonder what happens to the present analysis in the continuum limit. In particular, how does it connect with that of Leutwyler and Smilga? The short answer is that

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10 I thank Vicente Azcoiti and collaborators for stressing to me the importance of the presence of this infinite tower of sum-rules.
there is no direct connection, since the limits \( a \to 0 \) and \( N_{\text{site}} \to \infty \) do not commute when in the Aoki-phase. If one takes \( N_{\text{site}} \to \infty \) first, as I have throughout, one is always in the \( p \)-regime for the neutral pion, so that the vacuum manifold is \( SU(2)/U(1) \), while, with \( a \to 0 \) first (and at the same time sending \( m \to 0 \) so as to remain in the Aoki-phase), the manifold is \( SU(2) \). Another way of seeing the difference is to note that, if \( N_{\text{site}} \to \infty \) before \( a \to 0 \), then would-be zero modes are completely buried in the continuum of near-zero modes, while if \( a \to 0 \) first then the would-be zero modes lie below the continuum of near-zero modes.

One can, nevertheless, ask what happens if \( a \to 0 \) first. One still expects \( \langle C_0^2 \rangle_\epsilon = 0 \) (from \( \chi \)PT or from the properties of p.d.f.s), and must understand this result. The answer turns out to be that zero-mode contributions to both \( \langle C_0^2 \rangle_{\text{disc},\epsilon} \) and \( \langle C_0^2 \rangle_{\text{conn},\epsilon} \) conspire to cancel the contribution from the continuum of near-zero modes to \( \langle C_0^2 \rangle_{\text{conn},\epsilon} \). The cancellation occurs as long as one of the sum-rules of Leutwyler and Smilga holds. Thus one could obtain this sum-rule by enforcing \( \langle C_0^2 \rangle_\epsilon = 0 \). In fact, it is possible to obtain the whole set of higher-order sum-rules by enforcing the \( \chi \)PT relations between condensates of higher powers. This shows the close relation between the methods used here and those of Ref. [10].

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**APPENDIX A: SPECTRAL ASYMMETRY AND TOPOLOGICAL SUSCEPTIBILITY AT \( a \neq 0 \)**

This appendix provides a more detailed argument for the result (5.6) used in the main text for the spectral asymmetry of \( H_W \). The argument consists of two parts. The first aims to justify the approximate proportionality

\[
\langle |n_{\text{asym}}(m_0)|^2 \rangle \propto \langle Q_{\text{top}}(m_0)^2 \rangle \equiv V \chi_t(m_0),
\]  

(A1)

where \( \chi_t \) is the topological susceptibility, and the arguments \( m_0 \) indicate that all quantities are evaluated in the Aoki-phase. This proportionality is for fixed \( m_0 \), and thus concerns the dependence on \( a \) and \( V \). The second part of the argument gives a derivation of the
parametric form of the $\chi_t$ in the Aoki-phase using “Wilson fermion $\chi$PT” ($W\chi$PT) \[4, 23\]. Combining these two parts leads to the desired result.

From the work of Refs. \[13, 16, 17, 18\] we have a fairly clear picture of how the spectral asymmetry occurs. Given a configuration, one considers the spectrum of low-lying eigenvalues of the “valence” Hermitian Wilson-Dirac operator, $H_W(m_V)$, in which $m_0$ is replaced by the bare valence quark-mass $m_V$. One studies this spectrum as a function of $m_V$, starting at positive values and decreasing to $m_V \approx -1$. Based on the numerical results of Ref. \[18\], and subsequent theoretical work \[20, 24\], I assume that there is a “valence Aoki-phase” for a region of negative $m_V$. For positive $m_V$ the spectral asymmetry vanishes, but, once $m_V$ is negative and one enters the “supercritical region”, eigenvalues can cross zero. This means that, by the time one reaches the Aoki-phase, some spectral asymmetry can have built up, and numerical results indicate that this in fact happens \[18\]. The asymmetry increases as one moves through the Aoki-phase, and becomes almost independent of $m_V$ shortly after leaving the Aoki-phase. This approximate independence continues down to $m_V \approx -1$, and is due to a cancellation of modes crossing in both directions rather than an absence of crossings. The resulting spectral asymmetry for $m_V \approx -1$ is known to provide a robust definition of the topological charge of the configuration \[17\].

From the results of Ref. \[18\], this behavior appears to hold for a wide variety of ensembles, both quenched and unquenched. I assume here that it also holds for unquenched ensembles in which $m_0$ is in range leading to a dynamical Aoki-phase. If so, then, for a given $m_0$, $n_{\text{asym}}$ will approximately track $Q_{\text{top}}$ as $a$ and $V$ are varied, leading to the result (A1). Note that the proportionality constant between these two quantities will depend on $m_0$, i.e. on where one lies in the Aoki-phase. Indeed, the behavior described in the previous paragraph implies that $n_{\text{asym}}/Q_{\text{top}}$ is small near the upper boundary of the Aoki-phase (larger $m_0$) and close to unity at the lower boundary.

Further justification for the assumed proportionality comes from considering the physical extent of the eigenmodes at zero-crossing. According to Ref. \[18\], this typically decreases as $m_V$ is decreased.Crudely speaking, one can think of the crossings which occur before entering and within the Aoki-phase as corresponding to “lumps” of topological charge that extend over many lattice spacings, and survive the continuum limit. By contrast, those that occur after traversing the Aoki-phase are mostly lumps of size $\sim a$. Thus, if $m_V$ is within the Aoki-phase, the spectral asymmetry gives an approximate measure of that
part of $Q_{\text{top}}$ resulting from lumps of greater than some minimal size. Since the topological susceptibility in the continuum limit (appropriately regularized $[25]$) is determined by lumps of size $\sim 1/\Lambda_{\text{QCD}}$, it is plausible that this “truncated” or “coarse-grained” topological charge should lead to a susceptibility proportional to the exact result, and thus to Eq. (A1).

I now move to the second part of the argument. Accepting (A1), the next task is to determine the expected dependence of $\chi_t$ in the Aoki-phase on $a$ (and possibly $V$). Given some assumptions, this can be done using $W\chi$PT, generalizing the standard continuum $\chi$PT analysis $[10, 26]$. As a byproduct, the form of the dependence of $\chi_t$ on $m_0$ will also be obtained, but this does not carry over to $\langle |n_{\text{asym}}(m_V)|^2 \rangle$ because the proportionality constant in (A1) depends on $m_0$.

In the continuum analysis, one introduces the $\theta F\tilde{F}$ term into the action, rotates it into the quark mass matrix using an anomalous singlet axial rotation, and then evaluates $Z(\theta)$ using $\chi$PT. At leading order, and in the $p$-regime at large volume, $Z(\theta) = \exp[-V\chi_{\text{min}}^x(\theta)]$, where $\chi_{\text{min}}^x$ is the ($\theta$-dependent) minimum of the potential in the chiral Lagrangian. Then one has

$$\chi_t = \lim_{V \to \infty} -\frac{1}{V} \frac{\partial^2 \ln Z(\theta)}{(\partial \theta)^2}\bigg|_{\theta=0} = \frac{\partial^2 \chi_{\text{min}}^x(\theta)}{(\partial \theta)^2}\bigg|_{\theta=0}. \quad (A2)$$

To generalize this to include discretization effects, one must certainly include $O(a^2)$ corrections to the potential, for these contribute to the vacuum energy at leading order in $W\chi$PT. It is less clear, however, how to introduce $\theta$ into $W\chi$PT. One might consider adding a bare $\theta F\tilde{F}$ term to the lattice action, mapping this to the Symanzik action, and then into the chiral Lagrangian—i.e. following the standard steps in $W\chi$PT. Such a bare operator will, however, mix with lower ($\bar{\psi}\gamma_5\psi$) and higher ($\bar{\psi}\gamma_5\sigma_{\mu\nu}F_{\mu\nu}\psi$) dimension operators, leading respectively to $O(1/a)$ effects that need to be subtracted non-perturbatively $[27]$ and $O(a)$ discretization errors.

I think, however, that these complications do not occur here because the asymmetry that appears in Eq. (A1) is proportional to a $Q_{\text{top}}$ that is regulated in the ultraviolet. This precludes mixing with lower-dimensional operators. In other words, the definition $Q_{\text{top}} = n_{\text{asym}}(m_V \approx -1)$ gives a result that requires no subtractions. $Q_{\text{top}}$ will, however, have discretization errors. For example, using an improved Wilson-Dirac operator in the valence $H_V$ would lead to a different assignment of topological charge on some configurations. What I assume here is that this is an $O(a^2)$ error rather than an $O(a)$ one, because one is,
in effect, using valence overlap fermions to measure $Q_{\text{top}}$, and overlap fermions have only $O(a^2)$ errors.

What this discussion leads to is the assumption that, in order to calculate $\chi_t$, the appropriate potential to use in the Symanzik continuum effective action is

$$V_{\text{Symanzik}} \sim \bar{\psi}(m + i\mu\gamma_5\tau_3)\psi + ai\bar{\psi}\sigma \cdot F\psi + a^2(\bar{\psi}\psi)^2 + i\theta F\bar{F} + O(\theta a^2). \quad (A3)$$

Here I use a schematic notation in which all constants of $O(1)$ have been dropped, and I have only shown one of the possible forms of the chiral-symmetry-breaking four-fermion operators. I have also dropped terms of higher order in the chiral counting $m \sim a^2$. In words, my assumption is that the lattice $Q_{\text{top}}$ matches onto $\int F\bar{F} + O(a^2)$ in (A3). The $O(\theta a^2)$ terms will give rise to mass independent $O(a^2)$ corrections to $\chi_t$, which I will drop for now but restore at the end.

Given Eq. (A3) [minus the $O(\theta a^2)$ terms] the remainder of the analysis is straightforward. One first rotates $\theta$ into the fermionic terms, with each (scalar or pseudoscalar) bilinear picking up a factor of $\exp(i\theta\gamma_5/2)$.$^{11}$ One then matches to the chiral effective theory, obtaining the same form as for $\theta = 0$ except for the substitution $\Sigma \to e^{-i\bar{\theta}\Sigma}$, where $\bar{\theta} = \theta/2$. Thus the potential becomes

$$V^\chi(\Sigma) = -\frac{2B_0 f^2}{4} \text{Tr} \left(e^{i\bar{\theta} M\Sigma\dagger} + e^{-i\bar{\theta} M\dagger\Sigma}\right) + \frac{c_2}{16} \left[\text{Tr}(e^{-i\bar{\theta}\Sigma} + e^{i\bar{\theta}\Sigma\dagger})\right]^2$$
$$+ \frac{c_2'}{16} \left\{2\text{Tr} \left(e^{-i\bar{\theta} \Sigma} + e^{i\bar{\theta} \Sigma\dagger}\right)^2 - \left[\text{Tr}(e^{-i\bar{\theta}\Sigma} + e^{i\bar{\theta}\Sigma\dagger})\right]^2\right\}. \quad (A4)$$

Here I have absorbed the $O(a)$ term into the mass matrix $M = m + i\mu\tau_3$ in the usual way, which remains possible even when $\theta \neq 0$. Compared to Eq. (2.1) in the main text, there is an additional term, that proportional to $c_2' \sim a^2\Lambda_{\text{QCD}}^6$. This term vanishes when $\theta = 0$ due to the properties of $SU(2)$ matrices, but is non-vanishing when $\theta \neq 0$. Recall also that $2f^2B_0 = c_1/m$.

To determine $\chi_t$ using (A2) one must minimize $V^\chi$ with respect to variations in $\Sigma$. This assumes $\mu$ is kept non-zero while $V \to \infty$ so that we are in the $p$-regime. Inserting $\Sigma = \text{\ldots}$

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$^{11}$ It is possible that one can avoid the extended discussion given above by starting with $\theta$ inserted into the quark mass matrix of the lattice theory, following the work of Ref. [28]. I have not, however, pursued to resolve the issues of renormalization that arise in this approach.
exp(iθ_0 \hat{n} \cdot \vec{\tau})\) one finds, up to an irrelevant constant, that
\[
\mathcal{V} = -c_1 \cos \theta_0 \cos \bar{\theta} + c_1 (\mu/m) \sin \theta_0 n_3 \cos \bar{\theta} + c_2 \cos^2 \theta_0 \cos^2 \bar{\theta} + c'_2 (1 - \cos^2 \theta_0)(1 - \cos^2 \bar{\theta}).
\]
\[\text{(A5)}\]

Minimizing with respect to \(\theta_0\), and considering only infinitesimal \(\mu\), leads to
\[
\cos \theta_{0,\text{min}} = \frac{c_1 \cos \bar{\theta}}{2(c_2 \cos^2 \bar{\theta} - c'_2 \sin^2 \bar{\theta})},
\]
\[\text{(A6)}\]
\[
\mathcal{V}_{\text{min}}(\theta) = -\frac{c_1^2}{4c_2} + \theta^2 \frac{c'_2 [1 - (c_1/2c_2)^2]}{4} + O(\theta^4),
\]
\[\text{(A7)}\]

and thus
\[
\chi_t = \frac{c'_2 [1 - (c_1/2c_2)^2]}{2} + O(a^2 \Lambda_{\text{QCD}}^6) = \frac{c'_2 \sin^2 \theta_{0,\text{min}}}{2} + O(a^2 \Lambda_{\text{QCD}}^6).
\]
\[\text{(A8)}\]

One finds that the “calculable part” of \(\chi_t\) is determined by the new low-energy constant, \(c'_2\). I have also reinserted the \(O(a^2)\) term resulting from the \(O(\theta a^2)\) contributions to Eq. (A3).

The \(O(a^2)\) term is of the same size as the \(c'_2\) contribution, but does not depend on \(m_0\), being simply a discretization error in \(Q_{\text{top}}\) and not related to the alignment of the vacuum. The overall conclusion is thus that \(\chi_t \sim a^2 \Lambda_{\text{QCD}}^6\), so that on a typical configuration, \(|n_{\text{asy}}| \sim \sqrt{V\chi_t} \sim a\sqrt{V} \Lambda_{\text{QCD}}^3\). This is the result used in the main text.

Finally, I address what happens in the \(\epsilon\)-regime for the charged pions. Here one must include in the calculation of \(Z(\theta)\) the integral over the direction, \(\hat{n}\), of the condensate in the \(SU(2)/U(1)\) manifold. Following the method of Ref. [10] I find that this adds to \(V\chi_t\) a contribution proportional to \((\mu V \Lambda_{\text{QCD}}^3)^2\). In order to be in the \(\epsilon\)-regime, however, this contribution must have magnitude much smaller than unity. Thus it has no impact on the topological susceptibility when \(V \to \infty\).

**APPENDIX B: ALTERNATIVE FORMULATION OF CONSISTENCY CONDITIONS**

In this Appendix I describe an alternative, and arguably more natural, formulation of the conditions which must be satisfied by eigenvalue distributions in order that the standard Aoki-phase scenario remain valid. The formulation uses the microscopic spectral density, and the corresponding higher-order eigenvalue correlations. For the continuum Dirac operator, these are the quantities whose properties are universal in QCD-like theories, and governed
by random matrix theory. To define them one “zooms in” on the region of eigenvalues of size $\lambda \ll (a\Lambda_{\text{QCD}})/N_{\text{site}}$.\(^{12}\)

$$\rho^s_{1}(x) \equiv \rho(\lambda = \frac{x}{N_{\text{site}}}) . \tag{B1}$$

Thus $\rho^s_{1}(x)dx$ is the average total number of eigenvalues between $\lambda = x/N_{\text{site}}$ and $(x + dx)/N_{\text{site}}$. When expressed in terms of $x$, eigenvalues on a single configuration form a discrete set of levels, spaced by $\sim 1/\rho(0)$. One obtains a continuous distribution only after averaging over configurations, and the resulting distribution has structure (oscillations about $\rho(0)$) which is the remnant of the discrete levels. This is different from $\rho(\lambda)$, which, as noted in the main text, becomes a continuous function $\rho_{U}(\lambda)$ on a single configuration when $N_{\text{site}} \to \infty$. Furthermore, $\rho(\lambda)$ does not display the oscillations for small $\lambda$ seen in $\rho^s_{1}(x)$, since they get averaged out when $N_{\text{site}} \to \infty$. The essential point is that $\rho^s_{1}(x)$ contains extra information about the IR region that is lost in $\rho(\lambda)$.

I assume in the following that the lattice quark mass is chosen so that $\rho(0) \neq 0$, implying that one is in the Aoki-phase in the standard $\chi$PT description. The eigenvalues of interest, which I call the “IR eigenvalues”, are those for which $\rho(\lambda)$ is approximately constant, i.e. for which higher-order chiral corrections are small. This requires $|\lambda| \ll a\Lambda_{\text{QCD}}$, which translates into a maximum $x$ of magnitude $x_{\text{max}} = c(a\Lambda_{\text{QCD}})N_{\text{site}}$, with $c \ll 1$ a positive constant. Since $\rho^s_{1}(x)$ is on average a constant, the number of eigenvalues in the range $-x_{\text{max}} \leq x \leq x_{\text{max}}$ is

$$\int_{-x_{\text{max}}}^{x_{\text{max}}} dx \rho^s_{1}(x) \approx 2x_{\text{max}}\rho(0),$$

and in particular is proportional to $N_{\text{site}}$.

The distribution of the IR eigenvalues is encoded by $\rho^s_{1}(x)$, along with higher order correlation functions, $\rho^s_{k}(x_1, \ldots, x_k)$. The latter are standard quantities and I use the definitions given in Ref. \cite{29}, that, in particular, do not include the subtraction of the “connected part”. Thus, if the eigenvalues were completely uncorrelated, one would have, for example,

$$\rho^s_{2}(x_1, x_2) = \rho^s_{1}(x_1)\rho^s_{1}(x_2) - \delta(x_1 - x_2)\rho^s_{1}(x_1).$$

The second term is present because $\rho^s_{2}$ is a correlation between the eigenvalues of distinct eigenvectors. To simplify some of the following formulae, I also use correlation functions in which these kinematic correlations are removed, e.g.

$$\tilde{\rho}^s_{2}(x_1, x_2) \equiv \rho^s_{2}(x_1, x_2) + \delta(x_1 - x_2)\rho^s_{1}(x_1). \tag{B2}$$

\(^{12}\) Other scaling factors are also used in the continuum literature, e.g. including a factor of the condensate, $\Sigma \propto \rho(0)$, so that the eigenvalue spacing is of $O(1)$. I prefer not to do this since $\rho(0)$ is not a constant, but rather depends on the position in the Aoki-phase. Note also that some authors define $\rho(\lambda)$ without dividing by $N_{\text{site}}$, in which case an additional factor of $1/N_{\text{site}}$ is needed on the right-hand-side of eq. (B1).
Then for uncorrelated eigenvalues one has \( \bar{\rho}_k^s(x_1, \ldots, x_k) = \prod_{i=1,k} \rho_i^s(x_i) \) for all \( k \). Both the \( \rho_k^s \) and \( \bar{\rho}_k^s \) are symmetric under interchange of any two arguments. It also useful to note the volume dependence of the normalization of the \( \bar{\rho}_k^s \):

\[
\int_{-x_{\text{max}}}^{x_{\text{max}}} \left( \prod_{i=1,k} dx_i \right) \bar{\rho}_k(x_1, \ldots, x_k) \propto (N_{\text{site}})^k,
\]

which is consistent with the expectation that \( \bar{\rho}_k^s \) approaches a constant when all arguments have magnitudes much larger than \( 1/\rho(0) \).

In the continuum, the corresponding correlators are even functions of each \( x_i \) separately, allowing one to work only with \( x_i \geq 0 \). On the lattice, however, parity invariance of \( H_W \) implies only that the \( \rho_k^s \) do not change when all arguments change sign simultaneously, e.g.

\[
\rho_k^s(x_1, x_2, \ldots, x_k) = \rho_k^s(-x_1, -x_2, \ldots, -x_k).
\]

The same holds for the \( \bar{\rho}_k^s \). Thus, antisymmetric parts such as

\[
\Delta \bar{\rho}_2^s(x_1, x_2) \equiv \left[ \bar{\rho}_2^s(x_1, x_2) - \bar{\rho}_2^s(-x_1, x_2) \right]/2 = -\Delta \bar{\rho}_2^s(-x_1, x_2)
\]

need not vanish, unlike in the continuum. In fact, this particular quantity must be non-vanishing since it encodes the spectral asymmetry, which itself is non-zero (as discussed in the main text and in Appendix A):

\[
\langle n_{\text{asym}}^2 \rangle \equiv \langle (N_+ - N_-)^2 \rangle = 4 \int_0^{x_{\text{max}}} dx_1 dx_2 \Delta \bar{\rho}_2^s(x_1, x_2), \quad (B6)
\]

(Note that the integrals here are over positive \( x_i \) only.) We do, however, learn from Eq. (B6) that \( \Delta \bar{\rho}_2^s \) cannot tend to a constant for large \( |x_i| \), unlike \( \rho_2^s \) itself. This is because the integration area grows as \( N_{\text{site}}^2 \) while the integral grows only as \( \langle n_{\text{asym}}^2 \rangle \propto N_{\text{site}} \) from Eq. (A11). One possible behavior is that \( \Delta \bar{\rho}_2^s \) falls off for large \( x_i \), and this indeed is what is suggested by the discussion of the spectral asymmetry in the main text.

It is straightforward to convert the sum-rules given in the main text into constraints on the \( \rho_k^s \) and/or \( \bar{\rho}_k^s \). Results are simplified by defining (following continuum usage)

\[
\Sigma_0 = \frac{a^3}{Z_P} \sin \theta_0 f^2 B_0 = \pi \rho(0).
\]

The sum-rule (5.2) then becomes

\[
\int_{-x_{\text{max}}}^{x_{\text{max}}} dx \frac{\rho_1^s(x)}{x^2} = \frac{2}{3} \Sigma_0^2.
\]

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This has the same form as the first Leutwyler-Smilga sum-rule for QCD [10], except that \( 2/3 \) is replaced in QCD by \( 1/2(2 + |\nu|) \), with \( \nu \) the topological charge. One must also exclude exact zero-modes from \( \rho_1^s \) in the continuum. Since \( \rho_1^s(x) \) is symmetric, one could restrict the integral to positive values only (and divide the right-hand-side by two)—this is how the sum-rules are usually expressed in the continuum.

In this and subsequent sum-rules an implicit limit of \( N_{\text{site}} \rightarrow \infty \) has been taken. This removes the UV contribution to the integral (arising from the large \( x \) behavior, \( \bar{\rho}_1^s \propto (x/N_{\text{site}})^3 \)), so that the dominant contribution to the integral is from the IR region. Note also that the precise upper limit, \( x_{\text{max}} \), is then irrelevant.

The next sum-rule is obtained from Eq. (5.5), and is

\[
\int_{-x_{\text{max}}}^{x_{\text{max}}} dx_1 dx_2 \frac{\bar{\rho}_1^s(x_1, x_2)}{x_1 x_2} = 4 \int_0^{x_{\text{max}}} dx_1 dx_2 \frac{\Delta \bar{\rho}_1^s(x_1, x_2)}{x_1 x_2} = \frac{\Sigma_0^2}{3},
\]  

(B9)

The oddness of the integrand in both \( x_1 \) and \( x_2 \) picks out the antisymmetric part \( \Delta \bar{\rho}_1^s \). This means that this sum-rule has no continuum analog.

In the discussion given in Sec. V, the consistency of the Aoki phase required what might appear to be an artificial construct, namely an antisymmetry in \( \rho_U(\lambda) \), subleading as \( N_{\text{site}} \rightarrow \infty \), and yet contributing to the sum-rules due to its IR divergence. By contrast, the consistency conditions seem quite natural in the present formulation. The lattice symmetries allow a new quantity to be present, i.e. \( \Delta \bar{\rho}_1^s(x_1, x_2) \), a function which one expects to remain non-vanishing in the \( N_{\text{site}} \rightarrow \infty \) limit. Just as \( \rho_1^s \) needs to satisfy a consistency condition [eq. (B8)], it seems natural that the new function should too. Certainly from a mathematical point of view there should be no barrier to satisfying (B8), since one has a function to play with and the only other constraint is eq. (B6). One solution is the second example given in Sec. V in which \( \Delta \bar{\rho}_1^s \propto 1/\sqrt{x_1 x_2} \).

The pattern of one sum-rule for each new function continues at higher order. The sum rules are obtained from enforcing

\[
\langle C_0^{2n} \rangle^\epsilon = \langle C_3^{2n} C_0^{2n'} \rangle^\epsilon = 0 \quad \text{and} \quad \langle C_3^{2n} \rangle^\epsilon = \frac{1}{2n + 1} \langle (C_3)^p \rangle^{2n}
\]  

(B10)

for integer values of \( n, n' \), results that can be obtained from \( \chi PT \) or using probability distribution functions. In particular, combining the sum-rules for \( C_0^4, C_0^2 C_3^2 \) and \( C_3^4 \), one
finds

\[
\frac{4}{15} \Sigma^4_0 = \int_{-x_{\text{max}}}^{x_{\text{max}}} dx_1 dx_2 \frac{\rho^s_2(x_1, x_2)}{x_1^2 x_2^2}.
\]  
(B11)

\[
\frac{2}{15} \Sigma^4 = \int_{-x_{\text{max}}}^{x_{\text{max}}} dx_1 dx_2 dx_3 \frac{\rho^s_3(x_1, x_2, x_3)}{x_1 x_2 x_3^2}.
\]  
(B12)

\[
\frac{1}{5} \Sigma^4 = \int_{-x_{\text{max}}}^{x_{\text{max}}} dx_1 dx_2 dx_3 dx_4 \frac{\rho^s_4(x_1, x_2, x_3, x_4)}{x_1 x_2 x_3 x_4}.
\]  
(B13)

Note that it is simpler here to use the \( \rho^s_k \) than the \( \bar{\rho}^s_k \). The first constraint picks out the continuum-like, symmetric part of \( \rho^s_2 \), and indeed a result of similar form holds in the continuum. The other two constraints pick out parts of the three- and four-point correlators that vanish in the continuum, but need not vanish on the lattice. These are new, essentially independent, functions, and there is no barrier that I can see to their satisfying the new sum-rules.

In principle, one can continue this procedure to arbitrarily high order, and obtain an infinite set of sum-rules. This set is analogous to those that hold for each value of \( \nu \) in the continuum, except that on the lattice one has the additional functions (those odd under sign flips of a subset of the \( x_i \)) and corresponding additional sum-rules. In the continuum, these sum-rules have been solved to obtain the \( \rho^s_k \), and from them the distribution of individual eigenvalues (as reviewed in Ref. [22]). It is an interesting challenge to extend this analysis to the lattice theory.

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