Constraint on the low energy constants of Wilson chiral perturbation theory

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Wilson chiral perturbation theory (WChPT) is the effective field theory describing the long-distance properties of lattice QCD with Wilson or twisted-mass fermions. We consider here WChPT for the theory with two light flavors of Wilson fermions or a single light twisted-mass fermion. Discretization errors introduce three low energy constants into partially quenched WChPT at $\mathcal{O}(a^2)$, conventionally called W'_6, W'_7, and W'_8. The phase structure of the theory at nonzero a depends on the sign of the combination $2W'_6 + W'_8$, while the spectrum of the lattice Hermitian Wilson-Dirac operator depends on all three constants. It has been argued, based on the positivity of partition functions of fixed topological charge, and on the convergence of graded group integrals that arise in the ϵ regime of WChPT, that there is a constraint on the low energy constants arising from the underlying lattice theory. In particular, for $W'_6 = W'_7 = 0$, the constraint found is $W'_8 \leq 0$. Here we provide an alternative line of argument, based on mass inequalities for the underlying partially quenched theory. We find that $W'_8 \leq 0$, irrespective of the values of W'_6 and W'_7. Our constraint implies that $2W'_6 > |W'_8|$ if the phase diagram is to be described by the first-order scenario, as recent simulations suggest is the case for some choices of action.

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I. INTRODUCTION

Effective field theories such as chiral perturbation theory (ChPT) contain coefficients, usually called low energy constants (LECs), which are not determined by symmetry. If the matching between the high and low energy theories is nonperturbative, as is the case in the matching of QCD to ChPT, then the LECs must be determined either by experiment or by a nonperturbative method such as lattice QCD. One usually has no information on the LECs, other than a prediction for their order of magnitude based on naive dimensional analysis. It is sometimes possible, however, to constrain the signs of particular LECs based on the physics of the high-energy theory. For example, certain four-derivative terms in the chiral Lagrangian are constrained to be positive based on causality [1]. This argument has been generalized and applied widely in Ref. [2]. Another example concerns the chiral Lagrangian describing a lattice simulation at nonzero lattice spacing with a mixed action (different valence and sea-quark actions). It is found in Ref. [3] that, using generalized QCD mass inequalities [4], one finds a constraint on a combination of the LECs which arise due to discretization errors.

A further method of constraining LECs has recently been discovered in the context of calculating the low energy spectrum and eigenvalue properties of the lattice Hermitian Wilson-Dirac operator [5,6]. One line of argument is based on the positivity of the underlying two-flavor fermion determinant, which follows from the γ_5 Hermiticity of the Wilson-Dirac operator. Specifically, the partition function at fixed (odd) topology is positive in the underlying theory but is only positive in the effective theory [here partially quenched Wilson ChPT (PQWChPT)] if the LECs satisfy a constraint [6]. In the standard convention for LECs,[1] this constraint is $W'_8 \leq 0$ if $W'_6 = W'_7 = 0$.[2] Another line of argument notes that the partially quenched partition function for zero-momentum modes (which determines the leading order behavior in the ϵ regime) converges only if $W'_8 \leq W'_6 + W'_7$ [5,6].[3] We also note that a similar constraint (specifically, $W'_8 \leq 0$ independent of W'_6 and W'_7) was found earlier by one of us, based on the finding that the method for calculating the spectral density in infinite volume using PQWChPT only worked if the constraint held [9]. It was not clear, however, whether this was a fundamental constraint or simply a shortcoming of the method of calculation.

The constraints found in Refs. [5,6,9] imply an interesting corollary if one assumes that scaling at large N_c (number of colors) is a good guide at $N_c = 3$. In particular, since $W'_6/W'_8 \sim W'_7/W'_8 \sim 1/N_c$, this assumption would mean that one can ignore W'_6 and W'_7 to first approximation. Then the constraints imply that any discretization of Wilson fermions will have an Aoki phase for small enough physical quark mass. The other possible phase diagram—the first-order scenario [10]—would not occur. This is in apparent contradiction with the results of simulations using dynamical twisted-mass fermions, which find strong

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[1]Note that our convention for W'_j, which follows Ref. [7], differs in sign from that used in Refs. [5,6].

[2]Since these LECs appear at leading order in the appropriate power counting, they are independent of the renormalization scale.

[3]It may be possible to obtain further constraints from these or similar lines of argument [6,8].

evidence for the first-order scenario [11–20]. Of course, large N_c scaling may not be useful for $N_c = 3$, in which case the connection between the constraint and the phase scenario need not hold.

Given this situation, we think that it is important to find an alternative line of argument leading to such constraints. This is what we provide in the present note. In particular, we find that a generalization of the mass-inequality method of Ref. [3] constrains the LECs of WChPT.[4] Our constraint results from considering the twisted-mass generalization of Wilson fermions and comparing the quark-connected part of the neutral pion propagator to the charged pion propagator. A partially quenched setup is required to separate the quark-connected and disconnected contractions, and this is why it is the LECs of partially quenched WChPT which enter. We find $W_8' \leq 0$, independent of W_6' and W_7'.

The remainder of this note is organized as follows. In the following section we explain how partial quenching allows one to separately calculate the quark-connected part of the neutral pion correlator. In Sec. III we present the calculation of the quark-connected neutral pion "mass" at leading order in WChPT. We do so only at maximal twist, since this suffices to show the constraint. In Sec. IV we derive an inequality among quark-connected correlation functions, from which follows the above-noted constraint. We summarize and offer some concluding comments in Sec. V. We relegate some technical details to two appendixes, the first concerning the form of the condensate in the partially quenched theory, and the second extending the analysis of the main text from maximal to arbitrary twist.

II. USING PARTIAL QUENCHING TO SELECT QUARK-CONNECTED CORRELATORS

Our argument uses twisted-mass fermions [22,23], so we begin by recalling the salient features of this approach. In an unquenched theory, the quark Lagrangian takes the form

$$\mathcal{L}_q = \bar{q}_S(D_W + m_0 + i\mu_0\gamma_5\tau_3)q_S, \tag{1}$$

where q_S is an isodoublet of quark fields (corresponding to the up and down quarks), and D_W is the Wilson-Dirac operator. The subscript "S" indicates that these are sea quarks, appearing in the fermion determinant, as opposed to the valence quarks introduced below.[5] We refer to m_0 as the normal (bare) mass and μ_0 as the twisted (bare) mass. The following considerations do not depend on whether D_W is improved, or on the form of the gauge action, so we do not specify either. We will need only the property of "γ_5 Hermiticity":

$$\gamma_5 D_W \gamma_5 = D_W^\dagger. \tag{2}$$

When writing the Lagrangian in the form (1), we are using what is commonly called the "twisted basis," in which the mass, and not the Wilson term, is twisted.

In the continuum limit, a mass term $m + i\mu\gamma_5\tau_3$ can be rotated into a purely normal mass $m_q = \sqrt{m^2 + \mu^2}$ by an appropriate axial rotation. Thus the apparent breaking of flavor by the μ term is misleading—flavor is preserved for all μ. At nonzero lattice spacing, however, flavor is explicitly broken from $SU(2)$ to $U(1)$, leading to a splitting of the pion multiplet: $m_{\pi^\pm} \neq m_{\pi^0}$. As is well-known (and as will be seen explicitly in the following section) the splitting is of $\mathcal{O}(a^2)$.

The particular case of maximal twist corresponds to tuning $m_0 \to m_c$ such that the physical normal mass vanishes (or is, at least, sufficiently small compared to the twisted mass). There are a number of different tuning criteria that can be used, leading to results for physical quantities differing only at $\mathcal{O}(a^2)$. For discussion of these issues see Refs. [17,18,20,25–31]. All that matters here, however, is that a consistent criterion exists in which m_c is fixed, such as the one based on the partially conserved axial current mass used in practice in present simulations [18–20].

We will also need to know the quark-level operators which couple to the charged and neutral pions in the twisted basis. These are given, e.g., in Appendix A of Ref. [18]. The charged pions are created by

$$P^\pm = i\bar{q}_S\gamma_5\tau_\pm q_S \qquad \left[\tau_\pm = \frac{1}{\sqrt{2}}(\tau_1 \pm i\tau_2)\right] \tag{3}$$

(independent of twist angle), while the neutral pion is created at maximal twist by

$$S^0 = -\bar{q}_S q_S. \tag{4}$$

Thus the two-point correlators of the charged fields,

$$C^\pm(n) = \langle P^\mp(0)P^\pm(n)\rangle \tag{5}$$

(n labeling lattice sites), have only quark-connected contributions. For example,

$$C^+(n) = 2\langle \mathrm{tr}(\gamma_5 G(\mu)_{0,n}\gamma_5 G(-\mu)_{n,0})\rangle, \tag{6}$$

where the trace is over (implicit) color and Dirac indices, and the quark propagator is

$$G(\mu)_{0,n} = \left(\frac{1}{D_W + m_c + i\mu\gamma_5}\right)_{0,n}. \tag{7}$$

The neutral pion propagator, however, has both quark-connected and -disconnected contributions:

$$C^0(n) = \langle S^0(0)S^0(n)\rangle \tag{8}$$

$$= C^{0,\mathrm{conn}}(n) + C^{0,\mathrm{disc}}(n), \tag{9}$$

[4]The fact that mass inequalities can provide useful information in twisted-mass theories has also been noted in Refs. [8,21].

[5]Simulations using two doublets of dynamical twisted-mass fermions are also now being done, with the second such fermion describing the strange and charm quarks [20]. The arguments in this note apply equally well to such a setup, however, because the second doublet contains degrees of freedom that are heavy on the scale of the light up and down quarks. Thus the form of the chiral Lagrangian used in Sec. III is unchanged (although the values of the LECs will be different), and the argument for the mass inequalities in Sec. IV goes through unchanged. It is important in this regard that the determinant in such $N_f = 2 + 1 + 1$ simulations remains real and positive [24].

$$C^{0,\mathrm{conn}}(n) = -\langle \mathrm{tr}(G(\mu)_{0,n}G(\mu)_{n,0} + G(-\mu)_{0,n}G(-\mu)_{n,0})\rangle, \quad (10)$$

$$C^{0,\mathrm{disc}}(n) = \langle \mathrm{tr}(G(\mu)_{0,0} + G(-\mu)_{0,0}) \times \mathrm{tr}(G(\mu)_{n,n} + G(-\mu)_{n,n})\rangle. \quad (11)$$

In practice, the quark-connected part has a much better signal to noise ratio than the disconnected part, but improved techniques have allowed the computation of the latter with errors small enough that the mass of the neutral pion can be extracted [18].

What we are interested in here, however, is the quark-connected part of the correlator. Since this is measured with small errors (comparable to those for the charged correlator), it is worthwhile investigating whether it contains useful information. In the physical two-flavor theory one cannot separate the two Wick contractions. It is well-known, however, that if one considers the partially quenched (PQ) extension of the theory [32], then, by adding enough valence quarks, one can find correlation functions which pick out any desired Wick contraction. In the present case it suffices to add a single valence isodoublet q_V and the corresponding ghost quark isodoublet $\tilde{q}_V$. The Lagrangian for each of these quarks is the same as that for q_S [the twisted-mass Lagrangian (1)], except that $\bar{q}_S$ is replaced by $\tilde{q}_S^\dagger$ for the ghost quark.[6]

[6]This glosses over an important subtlety. In the ghost sector, convergence of the functional integral requires that the real part of the eigenvalues of the discretized fermion operator are positive. This is not the case for $D_W + m_0 + i\mu\tau_3\gamma_5$ given that one always works with $m_0 < 0$. This issue has been resolved, in the context of the quenched theory, in Ref. [33], and a simple generalization works here. The solution is to do an axial rotation in the τ_3 direction by angle $\pi/4$, such that the fermion operator becomes $D - i\gamma_5\tau_3(W + m_0) + \mu$, where D is the naive discretization of the Dirac operator and W the Wilson term. This new operator consists of an anti-Hermitian part, with purely imaginary eigenvalues, and a real offset μ, which we choose to be positive. (For negative μ, an axial rotation in the other direction resolves the problem.) For maximal twist, this is exactly the axial rotation that brings one to the physical basis, but for other twist angles it gives a different basis. In this new basis one can add in valence and ghost quarks. One then goes through the standard steps to obtain the chiral Lagrangian including discretization errors [10], following a simple generalization of the analysis of Ref. [33]. Compared to the usual chiral Lagrangian, one has additional factors of $\pm i\tau_3$ in terms containing spurions coming from discretization errors. Thus the Lagrangian looks nonstandard. In the quark sector (sea and valence) one can, however, undo the axial rotation (now at the level of the chiral fields) ending up with the standard form of the chiral Lagrangian for WChPT [presented below in Eq. (14)]. This does not work in the ghost sector, since one is not allowed to do normal axial rotations there. This restriction does not, however, effect the present calculation, since we only consider correlation functions in the quark sector. In fact, the correct procedure in the ghost sector has been worked out in Ref. [34], generalizing the methodology of Ref. [33].

Within this PQ setup, the correlation function which yields the quark-connected part of the neutral pion correlator involves the mixed valence-sea pion:[7]

$$C^{0,\mathrm{conn}}(n) = \langle \bar{q}_S q_V(0)\bar{q}_V q_S(n)\rangle. \quad (12)$$

This is because there is no disconnected Wick contraction between a $\bar{q}_S$ and q_V. Although we will not use it, it is perhaps of interest to note that the disconnected neutral pion Wick contraction can be obtained as

$$C^{0,\mathrm{disc}}(n) = \langle \bar{q}_S q_S(0)\bar{q}_V q_V(n)\rangle. \quad (13)$$

Partial quenching is often used to consider valence masses (or actions) differing from those of the sea quarks. In this work, by contrast, the valence and sea quarks have identical actions and masses. Thus there is an exact $SU(2)$ flavor symmetry mixing valence and sea quarks. This is a subgroup of the $SU(4)$ flavor symmetry that emerges in the continuum limit [itself a subgroup of the graded flavor group $U(4|2)$ that holds for perturbative calculations in the continuum PQ theory [35]].

We also remark that $C^{0,\mathrm{conn}}$ and $C^{0,\mathrm{disc}}$ are separately unphysical—they cannot be expressed in terms of a sum of exponentially falling terms with positive (real) coefficients. Nevertheless, they can be calculated using the appropriate low energy effective theory—PQWChPT—which itself is an unphysical theory, although perfectly well defined in Euclidean space. It turns out that $C^{0,\mathrm{conn}}$ does have, at leading order in WChPT, a physical form at long distances, which is all that we need for our argument.

III. WILSON CHPT CALCULATION OF CONNECTED PION MASSES

In this section we calculate $C^{0,\mathrm{conn}}$ and $C^{\pm}$ using PQWChPT. We are interested in the differences between these two correlators, which turn out to arise at $\mathcal{O}(a^2)$. Thus we work to leading order (LO) in the "large cutoff effects" or "Aoki" regime in which the power counting is $m \sim \mu \sim a^2\Lambda_{\mathrm{QCD}}^3$, where m and μ are the physical normal and twisted masses [defined in Eq. (16) below]. There is no need to work to higher order, since for the purposes of constraining the LECs we can imagine that m, μ, and a^2 are arbitrarily small.

At leading order, and after shifting the quark mass to remove an $\mathcal{O}(a)$ term, the partially quenched chiral Lagrangian is [7,10]

$$\mathcal{L}_\chi = \frac{f^2}{4}\mathrm{Str}(\partial_\mu\Sigma\partial_\mu\Sigma^\dagger) - \frac{f^2}{4}\mathrm{Str}(\chi^\dagger\Sigma + \Sigma^\dagger\chi) - \hat{a}^2 W_6'[\mathrm{Str}(\Sigma + \Sigma^\dagger)]^2 - \hat{a}^2 W_7'[\mathrm{Str}(\Sigma - \Sigma^\dagger)]^2 - \hat{a}^2 W_8'\,\mathrm{Str}(\Sigma^2 + [\Sigma^\dagger]^2). \quad (14)$$

[7]We could just as well add two isodoublets of valence quarks (and corresponding ghosts) and use $\langle \bar{q}_{V1}q_{V2}(0)\bar{q}_{V2}q_{V1}(n)\rangle$. The choice made in the text is, however, the minimal one.

Here $\Sigma \in SU(4|2)$, "Str" stands for supertrace, $\chi = 2B_0 M$ with M the mass matrix, and $\hat{a} = 2W_0 a$. B_0 and f are continuum LECs (with the convention $f_\pi \approx 93$ MeV), while W_0, W_6', W_7', and W_8' are LECs associated with discretization errors. Since our setup requires just two valence quarks and two ghosts, the graded chiral symmetry is[8] $SU(4|2)_L \times SU(4|2)_R$.

The mass matrix in $\mathcal{L}_\chi$ is related to the bare masses in the underlying quark Lagrangian (1). For the unquenched theory, we have

$$M = m + i\mu\tau_3 = m_q e^{i\omega_m \tau_3}, \tag{15}$$

$$m = Z_S^{-1}(m_0 - m_c)/a, \qquad \mu = Z_P^{-1}\mu_0/a. \tag{16}$$

Here ω_m is the "input" twist angle, and $m_q = \sqrt{m^2 + \mu^2}$ is the physical mass in the continuum limit. Maximal twist corresponds to $m = 0$. Note that in this case one does not need to know the renormalization factors Z_S and Z_P in order to determine the twist angle. For the partially quenched theory, the mass matrix, which has dimension 6×6, is block diagonal, with each block containing M. As noted in the previous section, this mass matrix leaves an unbroken $SU(2)$ symmetry between sea and valence quarks.

We must first determine the orientation of the vacuum, $\Sigma_0 = \langle 0|\Sigma|0\rangle$, taking into account the $\mathcal{O}(a^2)$ terms. In the unquenched sector this has been done in Refs. [36–38]. Writing

$$\Sigma_0^{\text{unqu}} = e^{i\omega_0 \tau_3}, \tag{17}$$

one needs in general to solve a quartic [given in Eq. (B1)] to determine ω_0, and $\omega_0 - \omega_m$ is generically of $\mathcal{O}(1)$. For the special case of maximal twist, however, the solution is simply $\omega_0 = \omega_m = \pm\pi/2$; i.e., the input and output twist angles are the same.

For the partially quenched theory, we argue in Appendix A that

$$\Sigma_0 = \begin{pmatrix} e^{i\omega_0\tau_3} & 0 & 0 \\ 0 & e^{i\omega_0\tau_3} & 0 \\ 0 & 0 & e^{\phi_g} \end{pmatrix}, \tag{18}$$

in a 2×2 block notation with the blocks ordered as sea, valence, and ghost quarks. In words, this result says that the $SU(2)$ valence-sea symmetry is unbroken (one implication of which is that the vacuum twist in the valence sector is the same as that in the sea sector) and that there are no quark-ghost condensates. We do not need to discuss the (subtle issue) of the ghost condensate e^{ϕ_g} (which is a 2×2 matrix), since we will not need propagators involving ghosts. This issue has been discussed, albeit in a different power counting, in Ref. [34].

Pion masses can now be obtained by considering small oscillations around the condensate. To do this, we use

$$\Sigma = \xi_0 \Sigma_{\text{ph}} \xi_0, \quad \xi_0 = \begin{pmatrix} e^{i\omega_0\tau_3/2} & 0 & 0 \\ 0 & e^{i\omega_0\tau_3/2} & 0 \\ 0 & 0 & e^{\phi_g/2} \end{pmatrix} \tag{19}$$

with $\Sigma_{\text{ph}} = \exp(i\sqrt{2}\pi/f)$ containing the pion fields. We will only need the quark part of the pion field, which we decompose as follows:

$$\mathcal{P}_q \pi \mathcal{P}_q = \begin{pmatrix} \pi_{SS} & \pi_{SV} & 0 \\ \pi_{VS} & \pi_{VV} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{20}$$

with $\mathcal{P}_q$ the projector onto the quark subspace

$$\mathcal{P}_q = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{21}$$

The block pion fields in (20) contain isosinglet components (i.e., η-like fields) as well as the usual isovector pions, but the isosinglet parts play no role in the following calculation. As we show below (following Ref. [39]), the symmetric positioning of the condensate in (19) leads to the usual identification of the individual pion fields in π. In particular, for the isovector fields, the decomposition for each block is the usual one,

$$\pi = \begin{pmatrix} \pi^0/\sqrt{2} & \pi^+ \\ \pi^- & -\pi^0/\sqrt{2} \end{pmatrix}. \tag{22}$$

To show this, we next need to map the operators $P^\pm$, S^0, and $\bar{q}_S q_V$ of Eqs. (3), (4), and (12) into the effective theory. This is a standard exercise, requiring the introduction of scalar and pseudoscalar sources into the mass matrix M. At LO in our power counting, the results are the same as in the continuum. In particular for quark bilinears we have

$$i\bar{q}T\gamma_5 q \longrightarrow -i\frac{f^2 B_0}{2}\,\text{Str}(\mathcal{P}_q T[\Sigma^\dagger - \Sigma]) \tag{23}$$

and

$$\bar{q}Tq \longrightarrow -\frac{f^2 B_0}{2}\,\text{Str}(\mathcal{P}_q T[\Sigma + \Sigma^\dagger]), \tag{24}$$

where T is an arbitrary flavor matrix acting on the 4×4 quark subspace. Using this result, and the expansion (19), we find

[8]The actual symmetry differs from this due to the constraints from convergence of ghost integrals. For perturbative calculations, such as those we perform here, one can, however, work as if the symmetry is as claimed. This was shown for the continuum PQ theory in Ref. [35], and presumably carries over to PQWChPT. In fact, all we need in the present calculation are fluctuations in the quark sector, and here the appropriate symmetry is certainly $SU(4)$. For nonperturbative calculations, however, such as those done in Refs. [5,6], one must account for the need to have convergent integrals in the ghost sector, which leads to a different global group.

$$P^{\pm} \longrightarrow -i\frac{f^2B_0}{2}\,\mathrm{Str}(\mathcal{P}^{SS}\tau_{\pm}[\Sigma_{\rm ph}^\dagger - \Sigma_{\rm ph}]) \tag{25}$$

$$= -2fB_0\pi_{SS}^{\mp} + \mathcal{O}(\pi^3), \tag{26}$$

$$S^0 \longrightarrow \frac{f^2B_0}{2}\,\mathrm{Str}(\mathcal{P}^{SS}\{c_0[\Sigma_{\rm ph} + \Sigma_{\rm ph}^\dagger] - is_0\tau_3[\Sigma_{\rm ph}^\dagger - \Sigma_{\rm ph}]\}) \tag{27}$$

$$= -s_0 2fB_0\pi_{SS}^0 + \mathcal{O}(\pi^2), \tag{28}$$

$$-\bar{q}_S q_V \longrightarrow \frac{f^2B_0}{2}\,\mathrm{Str}(\mathcal{P}^{SV}\{c_0[\Sigma + \Sigma^\dagger] - is_0\tau_3[\Sigma_{\rm ph}^\dagger - \Sigma_{\rm ph}]\}) \tag{29}$$

$$= -s_0 2fB_0\pi_{VS}^0 + \mathcal{O}(\pi^2). \tag{30}$$

where $c_0 = \cos\omega_0$ and $s_0 = \sin\omega_0$. $\mathcal{P}^{SS}$ is the projector onto the sea-sea block, and $\mathcal{P}^{SV}$ picks out the off-diagonal valence-sea block:

$$\mathcal{P}^{SS} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \mathcal{P}^{SV} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{31}$$

Thus, at maximal twist ($s_0 = 1$), $P^{\pm}$ and S^0 indeed couple with equal strength to the charged and neutral pions, respectively, as required by the underlying theory. We also see that π_{VS}^0 is the appropriate field to use to determine the connected part of the neutral correlator.

We can now calculate the correlators $C^{\pm}(x)$, $C^0(x)$, and $C^{0,\mathrm{conn}}(x)$ of Eqs. (5), (8), and (12), respectively.[9] At this stage we specialize to maximal twist. This not only simplifies the resulting expressions but also turns out, as sketched in Appendix B, to give the same constraint on the LECs as one finds when working at arbitrary twist. Expressed in terms of the rotated fields, the chiral Lagrangian becomes

$$\begin{aligned}\mathcal{L}_\chi = {}& \frac{f^2}{4}\,\mathrm{Str}(\partial_\mu\Sigma_{\rm ph}\partial_\mu\Sigma_{\rm ph}^\dagger) - \frac{f^2}{4}2B_0m_q\,\mathrm{Str}(\Sigma_{\rm ph} + \Sigma_{\rm ph}^\dagger)\\ &- \hat{a}^2W_6'[\mathrm{Str}(\Sigma_0\Sigma_{\rm ph} + \Sigma_0^\dagger\Sigma_{\rm ph}^\dagger)]^2\\ &- \hat{a}^2W_7'[\mathrm{Str}(\Sigma_0\Sigma_{\rm ph} - \Sigma_0^\dagger\Sigma_{\rm ph}^\dagger)]^2\\ &- \hat{a}^2W_8'\,\mathrm{Str}(\Sigma_0\Sigma_{\rm ph}\Sigma_0\Sigma_{\rm ph} + \Sigma_0^\dagger\Sigma_{\rm ph}^\dagger\Sigma_0^\dagger\Sigma_{\rm ph}^\dagger).\end{aligned} \tag{32}$$

Keeping only terms quadratic in the pion fields, we find that the W_6' term gives

$$-w_6'f^2(\pi_{SS}^0 + \pi_{VV}^0 + \text{ghost terms})^2, \tag{33}$$

the W_7' term vanishes, and the W_8' term becomes

$$-w_8'f^2(\tfrac{1}{2}[\pi_{SS}^0]^2 + \pi_{SV}^0\pi_{VS}^0 + \tfrac{1}{2}[\pi_{VV}^0]^2 + \text{ghost terms}). \tag{34}$$

Here we are using rescaled, dimensionless LECs

$$w_k' = \frac{16\hat{a}^2W_k'}{f^4} \qquad (k = 6, 7, 8). \tag{35}$$

We see that, while the W_8' term contributes to the masses of all the neutral pions, the W_6' term contributes only to the neutral particles in the diagonal blocks (and thus not to the π_{SV}^0 mass). This is because of the double-strace form of W_6', which means that it gives "hairpin vertices" in the usual PQChPT parlance.

Putting this all together, we find that, at leading order, each correlator of interest is proportional to the propagator of the corresponding pion. In momentum space we have (still at maximal twist)

$$\tilde{C}^j(p) = \frac{4f^2B_0^2}{p^2 + (m_\pi^j)^2}, \tag{36}$$

with $j = \pm$, 0, and "0, conn," where[10]

$$(m_\pi^{\pm})^2 = (m_{SS}^{\pm})^2 = 2B_0\mu, \tag{37}$$

$$(m_\pi^0)^2 = (m_{SS}^0)^2 = 2B_0\mu - (2w_6' + w_8')f^2, \tag{38}$$

$$(m_\pi^{0,\mathrm{conn}})^2 = (m_{SV}^0)^2 = 2B_0\mu - w_8'f^2. \tag{39}$$

The results for $m_{\pi^\pm}$ and m_{π^0} agree with those of Refs. [36–38], while that for the connected neutral pion is new. It is the latter result which provides the key constraint, as we now explain.

IV. MASS INEQUALITY AND THE CONSTRAINT ON LECS

We begin by rewriting the charged correlators using $\gamma_5G(-\mu)\gamma_5 = G(\mu)^\dagger$ (which follows from γ_5-Hermiticity):

$$C^+(n) = 2\langle\mathrm{tr}(G(\mu)_{0,n}G(\mu)_{n,0}^\dagger)\rangle, \tag{40}$$

$$C^-(n) = 2\langle\mathrm{tr}(G(\mu)_{0,n}^\dagger G(\mu)_{n,0})\rangle. \tag{41}$$

These two correlators are equal by charge conjugation symmetry, i.e., after averaging over each gauge field and its complex conjugate. Note that both correlators are a sum over positive definite terms, which leads us to expect that they are larger than all other correlators (assuming

[9]Note that we are now in a continuum theory, so the lattice label n is replaced by Euclidean position x (with the correspondence $x \sim an$).

[10]There is one subtlety in the calculation. As can be seen from Eq. (33), there are off-diagonal terms proportional to w_6' connecting π_{SS}^0 to π_{VV}^0 and ghost terms. These do not contribute, however, due to a cancellation between valence and ghost contributions, as must be the case because, for a purely sea-quark pion, we can do the calculation solely in the unquenched WChPT, leading to the result stated.

appropriate overall normalization factors). This is the basis for the mass-inequality method.

In the present case, we can adapt the argument given in Ref. [3]. We start by noting that, on each gauge configuration,

$$0 \leq |[G(\mu) + G(\mu)^\dagger]_{0a,nb}|^2 \tag{42}$$

$$= [G(\mu) + G(\mu)^\dagger]_{0a,nb}[G(\mu)^\dagger + G(\mu)]_{nb,0a}, \tag{43}$$

where a and b are color-Dirac indices. Multiplying out, summing over the color-Dirac indices, averaging over configurations (allowed since the quark determinant is real and positive), and using Eqs. (6) and (10), we arrive at the key inequality[11]

$$\frac{C^+(n) + C^-(n)}{2} = C^+(n) \geq C^{0,\mathrm{conn}}(n), \tag{44}$$

which holds for all n.

Now, for long distances, we can use the forms predicted by PQWChPT, which we know from the previous section to be (after Fourier transforming)

$$C^+(n) \propto (m^+_{SS})^{1/2}(an)^{-3/2}e^{-m^+_{SS}an}, \tag{45}$$

$$C^{0,\mathrm{conn}}(n) \propto (m^0_{SV})^{1/2}(an)^{-3/2}e^{-m^0_{SV}an}, \tag{46}$$

with a common coefficient of proportionality. We stress that, although $C^{0,\mathrm{conn}}$ is unphysical, PQWChPT predicts that it has a single-particle exponential falloff at long distances. The only way that (45) and (46) can be consistent with the inequality (44) for n large enough that the exponential damping dominates is if

$$m^+_{SS} \leq m^0_{SV} \tag{47}$$

or, equivalently,

$$m^\pm_\pi \leq m^{0,\mathrm{conn}}_\pi. \tag{48}$$

Combining this with the results for the masses from PQWChPT, Eqs. (37) and (39), we find that

$$w'_8 \leq 0 \Leftrightarrow W'_8 \leq 0. \tag{49}$$

As shown in Appendix B, one finds no other constraints on the LECs if one repeats the argument at nonmaximal twist.

The inequality (48) can be directly tested in lattice simulations, and present results (see, e.g., Fig. 6 of Ref. [18]) clearly satisfy the inequality.

[11]The correlators $C^\pm$ are real and positive, while $C^{0,\mathrm{cont}}$ is *a priori* only known to be real but of indeterminate sign. The PQWChPT result (36) shows, however, that at long distances $C^{0,\mathrm{cont}}$ is also positive. Thus we chose to consider the sum $G(\mu) + G(\mu)^\dagger$ in Eq. (42), so that $C^{0,\mathrm{conn}}$ would appear with a positive sign on the right-hand side of the inequality (44). We note for completeness, however, that we could also have considered the difference in $G(\mu) - G(\mu)^\dagger$ in Eq. (42), from which one would deduce that, in general, $C^+(n) \geq |C^{0,\mathrm{conn}}(n)|$.

We close this section by noting a relationship between the mass inequality (48) and the analysis of the condensate given in Appendix A. One of the conclusions from the appendix is that the sea-valence $SU(2)$ symmetry cannot be spontaneously broken for nonzero μ_0. This is consistent with the mass inequality because, if there were a mixed sea-valence condensate, then one would expect that fluctuations in the sea-valence direction would diverge, and thus that $(m^0_{SV})^2$ would pass through zero and become negative. The mass inequality says that this cannot happen while m^+_{SS} is positive, as it is expected to be for any nonzero μ_0.

V. CONCLUSIONS

We have shown that the sign of one of the LECs induced in Wilson ChPT by discretization errors can be determined by combining partially quenched WChPT with mass inequalities. The core of the argument is technically very simple, requiring only a tree-level computation and a simple inequality. The only connection between our argument and those given in Refs. [5,6] is that both require the positivity of the determinant.

The constraint we find is that $W'_8 \leq 0$, independent of the values of W'_6 and W'_7. We find no constraints on the latter two LECs. These results are the same as found in Ref. [9], based on the failure of a method to calculate the spectral density of the Hermitian Wilson-Dirac operator. Our constraint is also consistent with that given in Ref. [6] based on the positivity of the partition function in odd topological sectors ($W'_8 \leq 0$ if $W'_6 = W'_7 = 0$). It differs from that found using the convergence of the zero-mode partition function, namely, $W'_8 \leq W'_6 + W'_7$ [6]. Whether our result is stronger or weaker than this constraint depends on the signs of W'_6 and W'_7.

We stress that all arguments leading to constraints rely on the applicability of partially quenched ChPT. In our case, we work in the "p regime"—i.e., large volumes, with only small perturbations around the ground state—while Refs. [5,6] work in the ϵ regime in which the zero modes must be integrated over the entire group manifold.

Our calculation also provides a simple way of determining W'_8 using the result (valid at maximal twist, and generalized to arbitrary twist in Appendix B)

$$(m^{0,\mathrm{conn}}_\pi)^2 - (m^\pm_\pi)^2 = -w'_8 f^2 + \mathcal{O}(a^4, a^2 m^2_\pi) \tag{50}$$

$$= -\frac{16\hat{a}^2 W'_8}{f^2} + \mathcal{O}(a^4, a^2 m^2_\pi). \tag{51}$$

It appears from recent simulations with twisted-mass fermions (see, e.g., Refs. [18,19]) that this should give a fairly accurate determination. The only concern is whether the LO contribution will dominate. It would thus be interesting to extend the one-loop calculation of Refs. [40,41] to the partially quenched theory. It would also be interesting to compare results obtained using (51) with those from other recently proposed methods for determining W_8', which are based on using a mixed action [42] or on partially quenched pion scattering amplitudes [43].

We return now to the implications for the phase structure of unquenched twisted-mass fermions. As noted in the introduction, this depends on the sign of the combination of LECs, $2W_6' + W_8'$. If this combination is negative, then one is in the Aoki-phase scenario, which means that $m_\pi^\pm < m_\pi^0$ as long as $\mu_0 \neq 0$ [as can been seen from Eqs. (37) and (38)]. The results of Refs. [11–20], however, favor the first-order scenario, with $m_\pi^\pm > m_\pi^0$ for $\mu_0 \neq 0$. This means that $2W_6' + W_8' > 0$, which, combined with the inequality $W_8' \leq 0$, implies in turn that $2W_6' > |W_8'|$. There is nothing theoretically inconsistent with this possibility, but it is somewhat surprising given that $W_6'/W_8' \propto 1/N_c$ for large N_c.

A related implication of the presence of the first-order scenario is that quark-disconnected contributions play an important role. It is these contributions which, despite being suppressed by $1/N_c$, lower the neutral pion mass below that of the charged pion. This violation of large N_c counting (Zweig's rule) is superficially analogous to the situation with the η' in QCD. Here, however, the effect has the opposite sign,[12] and is of $\mathcal{O}(a^2)$ rather than a physical effect.

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APPENDIX A: FORM OF THE PARTIALLY QUENCHED CONDENSATE

In this appendix we present the arguments for the form of the condensate given in Eq. (18). The discussion is carried out in the underlying theory.

We first note that we know from a general argument given in Ref. [3] that quark-ghost condensates vanish. This leads to the zero entries in the rightmost column and bottom row (aside from the bottom-right block).

Second, we show that the valence-sea $SU(2)$ symmetry is unbroken, leading to the other zeros in (18), as well as the result that the condensate in the valence-valence block is the same as that in the sea-sea block. The argument is a generalization of the Vafa-Witten theorem on the absence of flavor breaking [45]. A similar argument was made in Ref. [3] concerning the absence of flavor breaking in the valence sector alone, but this was dependent on the fact that the valence sector contained quarks with an exact chiral symmetry, so that the Dirac operator has a continuumlike spectrum. In the present case we have valence and sea Wilson fermions, with no chiral symmetry, so the argumentation is different. In fact, it is surprising that one can make such an argument at all, since we know that the $SU(2)$ symmetry in the sea sector can be spontaneously broken—this is, after all, what happens in the Aoki phase. The key difference here is that we are working at nonvanishing twisted mass, which avoids the appearance of small eigenvalues of the Wilson-Dirac operator.

We show first that the sea-valence condensate

$$\langle \bar{q}_{Su} \gamma_5 q_{Vu} \rangle \tag{A1}$$

vanishes. The notation here is that, in each 2×2 block, we label the two states by u and d. Thus q_{Vu} is the valence u quark. We work in a volume V, at nonzero lattice spacing a, and with μ_0 nonzero. We turn on a source term

$$\mathcal{L}_{\text{source}} = \Delta \bar{q}_{Vu} \gamma_5 q_{Su}, \tag{A2}$$

chosen to "push" the condensate in a direction such that (A1) is nonzero. We then take $V \to \infty$, followed by $\Delta \to 0$, and find that (A1) vanishes. This implies the absence of spontaneous symmetry breaking.

Explicitly, a simple calculation yields (up to corrections proportional to Δ^3)

$$\frac{1}{V}\sum_n \langle \bar{q}_{Su} \gamma_5 q_{Vu}(n) \rangle = \frac{\Delta}{V}\left\langle \mathrm{Tr}\left(\gamma_5 \frac{1}{D_W + m_0 + i\mu_0\gamma_5} \gamma_5 \frac{1}{D_W + m_0 + i\mu_0\gamma_5}\right)\right\rangle \tag{A3}$$

$$= \frac{\Delta}{V}\left\langle \mathrm{Tr}\left(\frac{1}{Q + i\mu_0}\, \frac{1}{Q + i\mu_0}\right)\right\rangle \tag{A4}$$

$$= \Delta \int d\lambda \rho(\lambda) \frac{1}{(\lambda + i\mu_0)^2}. \tag{A5}$$

Here the traces are over space, Dirac, and color indices, $Q = \gamma_5(D_W + m_0)$ is the Hermitian Wilson-Dirac operator, which has (real) eigenvalues denoted by λ, and $\rho(\lambda)$ is the density of eigenvalues per unit volume after averaging over gauge fields. Note that we expect $\rho(0)$ to be nonvanishing in general (which gives rise to the Aoki phase [10,46]) but the presence of $\mu_0 \neq 0$ shields us from the potential singularity at $\lambda = 0$. Indeed, the coefficient multiplying Δ is finite for any nonzero a, since the range of the integration over λ is finite. Thus the sea-valence condensate vanishes when $\Delta \to 0$.

Note that to make this argument we need the eigenvalue density to be well defined, and for this we need the

[12] This point has been stressed recently in Ref. [44].

integration over gauge fields to have a positive weight, which is the case for twisted-mass fermions.

Similar arguments show that all the condensates $\langle \bar{q}_{Sj}\gamma_5 q_{Vk}\rangle$ vanish, with j and k running independently over u and d. Also, by using different twisted masses for valence and sea quarks one can show that condensates $\langle \bar{q}_{Sj}\gamma_5 q_{Sk} - \bar{q}_{Vj}\gamma_5 q_{Vk}\rangle$ vanish. For the corresponding scalar condensates, e.g., $\langle \bar{q}_{Sj} q_{Vk}\rangle$, one ends up with expressions such as

$$\frac{\Delta}{V}\left\langle \mathrm{Tr}\left(\gamma_5 \frac{1}{Q + i\mu_0}\gamma_5 \frac{1}{Q + i\mu_0}\right)\right\rangle. \quad \text{(A6)}$$

Although an eigenvalue decomposition cannot be used here, there is no reason to expect that the coefficient of Δ diverges for nonzero a, given the presence of $\mu_0 \neq 0$. Assuming so, we find that all sea-valence condensates vanish.

APPENDIX B: CONNECTED PION MASSES AT ARBITRARY TWIST ANGLE

In this appendix we give the values of the masses $(m_\pi^\pm)^2$, $(m_\pi^0)^2$, and $(m_\pi^{0,\mathrm{conn}})^2$ at arbitrary twist angle. For a lattice theory in the large cutoff effects regime, if the mass twist angle ω_m is not an integer multiple of $\pi/2$, then it will differ from the twist angle in the condensate, ω_0. As a result, when the leading order chiral Lagrangian is expressed in the physical basis (in terms of Σ_{ph}), the form of both the mass term and the $\mathcal{O}(a^2)$ terms is altered by the twist. Expanding the leading order chiral Lagrangian to $\mathcal{O}(\pi^2)$, one fixes the relation between ω_m and ω_0 by demanding that the linear term vanish. This relation is the same as in the unquenched case [36–38]:

$$2B_0\mu \sin(\omega_0 - \omega_m) = -f^2(2w_6' + w_8')s_0 c_0. \quad \text{(B1)}$$

This can be used to rewrite the quadratic terms in $\mathcal{L}_\chi$ so that they depend only on ω_0 and not ω_m. One may then read off the masses

$$(m_\pi^\pm)^2 = \frac{2B_0\mu}{s_0}, \quad \text{(B2)}$$

$$(m_\pi^0)^2 = \frac{2B_0\mu}{s_0} - f^2(2w_6' + w_8')s_0^2, \quad \text{(B3)}$$

$$(m_\pi^{0,\mathrm{conn}})^2 = \frac{2B_0\mu}{s_0} - f^2 w_8' s_0^2. \quad \text{(B4)}$$

The results for the unquenched charged and neutral pions agree with those of Refs. [37,39].

By generalizing the arguments of Sec. IV one can show that the connected neutral mass can be no smaller than the charged mass. We sketch the generalization briefly. The form of the charged correlator, Eq. (6), is independent of twist. The neutral correlator does, however, depend on twist; the operator used to create the neutral sea-valence pion becomes

$$\bar{q}_S i\gamma_5\tau_3 e^{i\gamma_5\tau_3\omega} q_V. \quad \text{(B5)}$$

Here ω is the twist angle determined in the simulation, from either the input masses or using one of the other possible definitions. It will not matter which definition is used, since the inequality holds independent of ω. Thus the connected neutral correlator becomes

$$C_\omega^{0,\mathrm{conn}}(n) = -\langle \mathrm{tr}(i\gamma_5 e^{i\gamma_5\omega}G(\mu)_{0,n} i\gamma_5 e^{i\gamma_5\omega}G(\mu)_{n,0} + i\gamma_5 e^{-i\gamma_5\omega}G(\mu)^\dagger_{0,n} i\gamma_5 e^{-i\gamma_5\omega}G(\mu)^\dagger_{n,0})\rangle. \quad \text{(B6)}$$

Now, using

$$|[-G(\mu)i\gamma_5 e^{i\gamma_5\omega_0} + i\gamma_5 e^{-i\gamma_5\omega_0}G(\mu)^\dagger]_{0a,nb}|^2 \geq 0, \quad \text{(B7)}$$

and following similar steps as in the main text, one finds that

$$C_\omega^{0,\mathrm{conn}}(n) \leq C^+(n). \quad \text{(B8)}$$

We stress that this inequality holds separately at each value of the input bare masses m_0 and μ_0, and furthermore, for fixed m_0 and μ_0, it holds for any choice of ω. When we evaluate the correlators in WChPT it is most natural to choose $\omega = \omega_0$, for then the connected neutral correlator couples to the sea-valence neutral pion with the same strength as the charged correlator does to the charged pion.[13] This means that the WChPT result Eq. (36) still holds, except that the masses which appear are now those of Eqs. (B2)–(B4) above.

Putting this all together, it follows that

$$(m_\pi^{0,\mathrm{conn}})^2 - (m_\pi^\pm)^2 = -f^2 w_8' s_0^2 + \mathcal{O}(a^3) \geq 0. \quad \text{(B9)}$$

Thus, on the one hand, the result $W_8' \leq 0$ can be demonstrated using any nonzero twist angle, but on the other, working at arbitrary twist does not provide an additional constraint on the LECs.

[13] Using other values of ω leads to a weaker inequality.

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