Phase diagram of twisted mass lattice QCD

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We use the effective chiral Lagrangian to analyze the phase diagram of two-flavor twisted mass lattice QCD as a function of the normal and twisted masses, generalizing previous work for the untwisted theory. We first determine the chiral Lagrangian including discretization effects up to next-to-leading order (NLO) in a combined expansion in which $m_\pi^2/(4\pi f_\pi)^2 \sim a\Lambda$ (a being the lattice spacing, and $\Lambda = \Lambda_{\mathrm{QCD}}$). We then focus on the region where $m_\pi^2/(4\pi f_\pi)^2 \sim (a\Lambda)^2$, in which case competition between leading and NLO terms can lead to phase transitions. As for untwisted Wilson fermions, we find two possible phase diagrams, depending on the sign of a coefficient in the chiral Lagrangian. For one sign, there is an Aoki phase for pure Wilson fermions, with flavor and parity broken, but this is washed out into a crossover if the twisted mass is nonvanishing. For the other sign, there is a first order transition for pure Wilson fermions, and we find that this transition extends into the twisted mass plane, ending with two symmetrical second order points at which the mass of the neutral pion vanishes. We provide graphs of the condensate and pion masses for both scenarios, and note a simple mathematical relation between them. These results may be of importance to numerical simulations.

I. INTRODUCTION AND CONCLUSION

There has been considerable recent interest in the twisted mass formulation of lattice QCD (tmLQCD).[1] This formulation has several significant advantages compared to "untwisted" Wilson fermions: first, the twisted mass provides an infrared cutoff for small eigenvalues of the lattice Dirac operator and thus avoids so-called exceptional configurations [2,3]; second, for maximal twisting (i.e., a purely twisted mass term) physical quantities are automatically O(a) improved [4]; and, finally, calculations of weak matrix elements are considerably simplified [3,5,6]. It may thus serve, for practical simulations, as an intermediate formulation between improved staggered fermions (which share the above advantages, but have the disadvantage of taking the square- or fourth-root of the fermion determinant) and chiral lattice fermions (which are more computationally expensive).

We consider here simplest version of tmLQCD which, by construction, is equivalent in the continuum limit to QCD with two degenerate flavors. At nonzero lattice spacing, however, the flavor group is explicitly broken from SU(2) down to U(1). This flavor breaking is analogous to the "taste symmetry" breaking of staggered fermions that plays a major role in practical simulations. It is thus important to study the impact of flavor breaking in simulations of tmLQCD. This can be done analytically using the chiral effective theory including the effects of discretization. The methodology for doing so for Wilson fermions was worked out in Ref. [7]. Here we provide the generalization to tmLQCD, determining the chiral effective Lagrangian to next-to-leading order (NLO). This extends the work of Ref. [8] by including terms proportional to a^2 (a being the lattice spacing).

There are many possible applications of the resulting effective Lagrangian. In this paper we focus on the phase structure. We extend the analysis of Ref. [7] (and the similar considerations of Ref. [9]) into the twisted mass plane. For untwisted Wilson fermions, Ref. [7] found two possibilities as the (untwisted) quark mass approaches the critical mass. In the first, the pion mass vanishes, and the theory enters an Aoki phase, in which flavor and parity are spontaneously broken. This is the scenario proposed long ago by Aoki [10–12], and supported by results from quenched simulations. The phase has width $\Delta m \sim a^2$, in terms of the physical quark mass m. The second possibility is that there is a first order transition at which the condensate flips sign, and the pion mass reaches a minimum, but is nonvanishing. In this scenario flavor and parity are unbroken. The choice of scenario is determined by the sign of a particular coefficient in the chiral Lagrangian [the coefficient is c_2 defined in Eqs. (35) and (37)], the value of which depends on the gauge action and the coupling constant. Indeed, numerical work with unquenched Wilson fermions [13] finds evidence for an Aoki phase at strong coupling (consistent with the expectations of analytic results in the strong coupling, large N_c limit [10]), but also finds that the phase disappears as the coupling is weakened. This suggests that the second scenario applies for moderate and weak couplings, at least with the Wilson gauge action. This conclusion is supported by the very recent work of Ref. [14], who find clear evidence of a first order transition along the Wilson axis.

The extension of the analysis of Ref. [7] into the twisted mass plane turns out to be relatively straightforward. The twisted mass introduces only a single additional term in the potential, one that attempts to twist the condensate in the direction of the full mass. We find that any nonzero value for the twisted mass washes out the Aoki phase of the first scenario, as expected when the would-be spontaneously broken symmetry is explicitly broken. Thus the Aoki phase itself is confined to a short segment of the untwisted axis, as shown in Fig. 1(a).
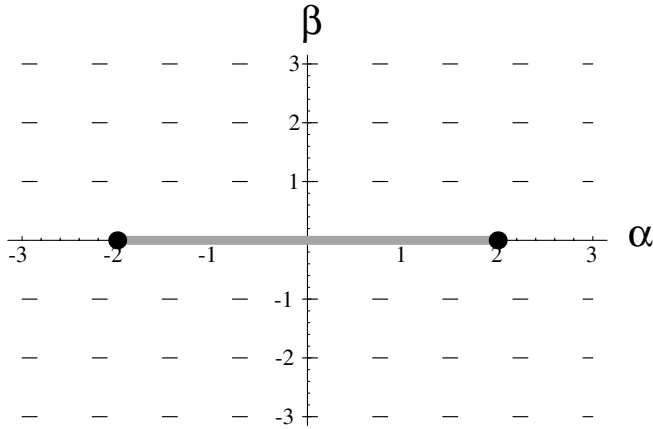
(a) Phase diagram for $c_2 > 0$
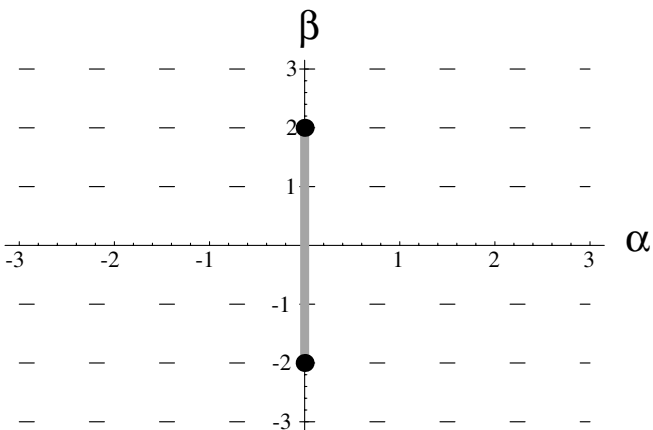
(b) Phase diagram for $c_2 < 0$

FIG. 1. Phase diagram of tmLQCD. α and β are proportional to the untwisted and twisted mass, respectively, in units proportional to the lattice spacing squared [see Eqs. (28),(29)]. The sign of the coefficient c_2 determines whether flavor symmetry is spontaneously broken in the standard Wilson theory. The solid lines are first order transitions across which the condensate is discontinuous, with second order endpoints. Figs. 2–4 show the dependence of the condensate and pion masses along the horizontal dashed lines. See text for further discussion.

Traversing this segment in the twisted direction there is a first order transition, with a discontinuity in the chiral condensate. More interesting, and, in light of the results of simulations noted above, probably more relevant, is the impact of twisting on the scenario with a first order transition. Here we find that the transition extends a distance of size $\Delta\mu \sim a^2$ (where μ is the physical twisted mass) into the plane, as shown in Fig. 1(b). The transition weakens as $|\mu|$ increases, ending with second order points where the neutral pion mass vanishes.

Looking at the phase diagram, the two scenarios appear related by a 90° rotation. In fact, this relation is exact for the condensate and the neutral pion mass, aside from corrections of $O(a^3)$ in the chiral effective theory. In other words, approaching the critical mass along the twisted mass axis the neutral pion mass has exactly the same dependence on the twisted mass as it does on the normal mass in an untwisted Wilson simulation *with the opposite value of* c_2. Similarly, the condensates in the two cases are simply related by a 90° twist. This identity does not, however, hold for the charged pion masses. These vanish in the Aoki phase, but do not vanish along the first order transition line for $c_2 < 0$. Nevertheless, there is still a simple relation between the two scenarios: the charged pion mass-squareds for $c_2 < 0$ are obtained from those for $c_2 > 0$ by rotating by 90° and then adding a constant positive offset (proportional to $|c_2|a^2$).

The possible presence of phase structure extending in the twisted mass direction may hinder numerical simulations—there would be premature critical slowing down due to the second order endpoint, and metastability beyond [14]. One can reduce these effects either by working at weaker coupling (since $\Delta\mu \propto a^2$), or by attempting to find a gauge action which gives rise to a smaller value of c_2.

The rest of this paper is organized as follows. In the next section, we present the two-step process of obtaining an effective chiral theory that describes the long distance physics of the underlying lattice theory of tmLQCD including discretization effects. We then, in Sec. III, explain how to use the resulting chiral Lagrangian to investigate the phase diagram of tmLQCD.

An partial account of the work presented here was given in Ref. [15]. Results on the masses and decay constants of pions will be presented elsewhere [16].

Similar conclusions have been reached independently by Münster [17,18] and Scorzato [19].

II. EFFECTIVE CHIRAL THEORY

The theory we consider here is tmLQCD with a doublet of degenerate quarks.[2] In this section, we start by briefly reviewing the symmetry properties of the tmLQCD ac-

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[2]We do not consider the generalization to nondegenerate quarks discussed in Ref. [20].

tion. We obtain the effective chiral theory for pions by first determining the effective continuum Lagrangian at the quark level and then matching it onto the chiral Lagrangian.

A. Twisted mass lattice QCD

The fermionic part of the Euclidean lattice action has the form [3,4]

$$S_F^L = a^4 \sum_x \bar\psi_l(x)\left[\frac{1}{2}\sum_\mu \gamma_\mu(\nabla_\mu^\star + \nabla_\mu)\right.$$
$$\left. - r\frac{a}{2}\sum_\mu \nabla_\mu^\star \nabla_\mu + m_0 + i\gamma_5\tau_3\mu_0\right]\psi_l(x), \quad (1)$$

where ψ_l and $\bar\psi_l$ are the bare lattice fields (with "l" standing for lattice and not indicating left-handed), and ∇_μ and $\nabla_\mu^\star$ are the usual covariant forward and backward lattice derivatives, respectively. The bare normal mass, m_0, and the bare twisted mass, μ_0, are taken to be proportional to the identity matrix in flavor space. A

possible "twist" in the Wilson term has not been included because it can be rotated away by appropriate changes in m_0 and μ_0. This means that we are using the so-called "twisted basis", which we find simplifies the subsequent analysis. We will not need to specify the irrelevant parameter r in our analysis, other than that it should be a nonvanishing constant, satisfying $|r| \leq 1$ for reflection positivity [4]. What we have in mind is the value $r = 1$ used in most numerical simulations.

The action given in (1), combined with any hypercubically invariant gluon action, shares the following symmetries with standard Wilson fermions: invariance under gauge transformations, lattice rotations and translations, charge conjugation, and the U(1) transformations associated with fermion number. It differs from standard Wilson fermions in two important ways. First, the flavor SU(2) symmetry is broken explicitly by the μ_0 term down to the U(1) subgroup with diagonal generator τ_3. Second, ordinary parity $\mathcal{P}$ is only a symmetry if combined either with a discrete flavor rotation

$$\mathcal{P}_F^{1,2} : \begin{cases} U_0(x) \to U_0(x_P), \qquad U_k(x) \to U_k^\dagger(x_P - a\hat k), \qquad k = 1, 2, 3, \\ \psi_l(x) \to i\gamma_0\tau_{1,2}\psi_l(x_P), \\ \bar\psi_l(x) \to -i\bar\psi_l(x_P)\tau_{1,2}\gamma_0, \end{cases} \quad (2)$$

[where $x_P = (-\mathbf{x}, t)$, and our generators are normalized as $\tau_i^2 = 1$], or combined with a sign change of the twisted mass term

$$\tilde{\mathcal{P}} \equiv \mathcal{P} \times [\mu_0 \to -\mu_0]. \quad (3)$$

The additional symmetries called $\mathcal{R}_5^{\text{sp}}$ and $\mathcal{R}_5 \times \mathcal{D}_d$ in Ref. [4] will not be needed here.

B. Effective continuum Lagrangian at the quark level

Following the program of Symanzik [21,22], the long distance properties of tmLQCD can be described by an effective continuum Lagrangian of the form:

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_0 + a\mathcal{L}_1 + a^2\mathcal{L}_2 + \cdots. \quad (4)$$

The key constraint is that this Lagrangian need only be invariant under the symmetries of the lattice theory. We will work through the terms in turn, emphasizing the differences that are introduced by the twisted mass. The analysis parallels and extends that of Ref. [7].

We consider first $\mathcal{L}_0$, which consists of operators of dimension four or less, and is the Lagrangian which survives in the continuum limit. The lattice symmetries restrict its form to be

$$\mathcal{L}_0 = \mathcal{L}_g + \bar\psi\left(\slashed{D} + Z_m\frac{m_0}{a} + i\gamma_5\tau_3\mu\right)\psi - Z_m\frac{\tilde m_c}{a}\bar\psi\psi, \quad (5)$$

where $\mathcal{L}_g$ is the continuum gluon Lagrangian, and, as discussed below, $\mu \propto \mu_0$. In particular, the parity-flavor symmetry $\mathcal{P}_F^{1,2}$ requires parity and flavor to be violated in tandem: it forbids the flavor singlet parity violating terms $\bar\psi\gamma_5\psi$ and $\tilde F_{\mu\nu}F_{\mu\nu}$, as well as the flavor violating, parity even operator $\bar\psi\tau_3\psi$. The residual flavor U(1) symmetry forbids bilinears containing the flavor matrices $\tau_{1,2}$. The coefficients Z_m, μ and m_c must be real in order to retain reflection positivity. Finally, the spurionic symmetry $\tilde{\mathcal{P}}$ implies that the flavor-parity violating operator $\bar\psi\gamma_5\tau_3\psi$ comes with a coefficient odd in μ_0, here of linear order.

The net effect is that the result (5) differs from that for Wilson fermions only by the μ term. In particular, the twisted mass is only multiplicatively and not additively renormalized [3].

The relationship between the parameters in the continuum Lagrangian and those in the bare lattice Lagrangian has been given in Ref. [3]. The continuum fields ψ are related to the bare lattice fields as follows:

$$\psi = a^{-3/2}Z[g^2(a), \ln(\Lambda_{\text{reg}}a)]\psi_l, \quad (6)$$

where Z is a matching factor, and Λ_{reg} is the renormal-

ization scale of the continuum theory. The physical quark mass is defined in the usual way,

$$m = Z_m(m_0 - \tilde{m}_c)/a, \qquad (7)$$

while the physical twisted mass is related to the bare parameters as

$$\mu = Z_\mu \mu_0/a = Z_P^{-1}\mu_0/a, \qquad (8)$$

with Z_P is the matching factor for the pseudoscalar density. Finally, the coupling constants in the continuum and lattice theories are related in the standard way. All the renormalization factors depend on $g^2(a)$ and, due to their anomalous dimensions, on $\ln(\Lambda_{\mathrm{reg}}a)$. We keep this (weak) dependence on the lattice spacing implicit. It should be borne in mind, however, that when, in the following, we refer to a power-law dependence on a, there will always be implicit subleading logarithmic corrections. We also note that the Z factors are mass-independent (assuming that we are using a mass-independent regularization scheme in the continuum) and thus are the same for the twisted mass theory as for normal Wilson fermions. The same is true of $\tilde{m}_c$.

In terms of the physical parameters, we finally have

$$\mathcal{L}_0 = \mathcal{L}_g + \bar{\psi}(\slashed{D} + m + i\gamma_5\tau_3\mu)\psi. \qquad (9)$$

In this theory, unlike on the lattice, the apparent flavor and parity breaking is fake, as μ can be rotated away by a nonanomalous axial rotation. This theory is thus equivalent to the usual, untwisted, two-flavor QCD with a mass $m' = \sqrt{m^2 + \mu^2}$.

We next construct $\mathcal{L}_1$, which contains dimension five operators. The enumeration of these operators is similar to that carried out in Ref. [23], and we find

$$\begin{aligned}
\mathcal{L}_1 = \; & b_1\bar{\psi}i\sigma_{\mu\nu}F_{\mu\nu}\psi + b_2\bar{\psi}(\slashed{D} + m + i\gamma_5\tau_3\mu)^2\psi \\
& + b_3m\bar{\psi}(\slashed{D} + m + i\gamma_5\tau_3\mu)\psi + b_4m\mathcal{L}_g \\
& + b_5m^2\bar{\psi}\psi + b_6\mu\bar{\psi}\{(\slashed{D} + m + i\gamma_5\tau_3\mu), i\gamma_5\tau_3\}\psi \\
& + b_7\mu^2\bar{\psi}\psi. \qquad (10)
\end{aligned}$$

The coefficients b_i must be real for reflection positivity, and have a similar implicit weak dependence on a as do the Z factors discussed above. Note that the form of $\mathcal{L}_1$ is similar to that for untwisted Wilson fermions [7], except for the inclusion of the twisted mass in the operator ($\slashed{D} + m + i\gamma_5\tau_3\mu$), and the addition of the b_6 and b_7 terms.

A number of potential terms have been excluded by the $\tilde{\mathcal{P}}$ symmetry: $m\mu\bar{\psi}\psi$, $m^2\bar{\psi}i\gamma_5\tau_3\psi$, $\mu^2\bar{\psi}i\gamma_5\tau_3\psi$, $\bar{\psi}D^2i\gamma_5\tau_3\psi$ and $\bar{\psi}i\sigma_{\mu\nu}F_{\mu\nu}i\gamma_5\tau_3\psi$. The last of these, the "twisted Pauli term", requires a factor of μ and thus appears only in $\mathcal{L}_2$. Charge conjugation symmetry enters at O(a), forbidding a term similar to that with

coefficient b_6 but containing a commutator instead of an anticommutator.

We can simplify $\mathcal{L}_1$ by dropping terms that vanish by the leading order equation of motion, i.e., that which follows from $\mathcal{L}_0$. This is equivalent to changing quark variables by an amount proportional to a. It removes the b_2, b_3 and b_6 terms.[3]

The situation with the b_4, b_5 and b_7 terms is more subtle. On the one hand, they can be removed by O(a) redefinitions of the parameters in $\mathcal{L}_0$ (the coupling constant for b_4, and the untwisted mass for b_5 and b_7). Note that for b_7 this is an additive redefinition ($m \to m + b_7a\mu^2$) which leads to a curvature in the critical mass m_c as a function of the twisted mass. On the other hand, when one makes such a redefinition one loses direct contact with the underlying bare parameters, which are linearly related to g, m and μ as explained above. If one wants to map out the phase diagram in terms of bare parameters, which is what one does in a numerical simulation, one should keep the b_4, b_5 and b_7 terms.

At this point, however, it is useful to anticipate the power-counting scheme that we use in our chiral effective theory. We consider m/Λ, μ/Λ and $a\Lambda$ as small quantities of the same size, and work to quadratic order in a combined chiral-continuum expansion. In this power-counting the three terms in question are all of cubic order, and can be dropped, avoiding the choice discussed in the previous paragraph. That the b_5 and b_7 terms are of cubic order is manifest, since they involve two powers of quark masses in addition to the overall factor of a multiplying $\mathcal{L}_1$. The b_4 term appears to be only of quadratic order, since it involves only a single power of the quark mass. However, this is a *relative* correction to a leading order term, and the leading order terms in the chiral effective theory are themselves of linear order. Thus its contributions to the effective theory are of cubic order.

Since we are working to quadratic order in the joint chiral-continuum expansion, we need to determine the form of $\mathcal{L}_2$, which contains dimension six operators. There are three such purely gluonic operators [24,25]. We do not write these down since, as explained in Ref. [26], they will lead to terms of too high order in our expansion. In particular, those which do not break the continuum rotation symmetry give rise to relative corrections proportional to a^2. Since the leading term in the chiral-continuum expansion is of O(m, a), these corrections are of cubic order and can be dropped. There are also gluonic operators which break the rotation symmetry

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[3]This is not strictly necessary. Terms vanishing by the equations of motion break the continuum symmetries in the same way as other terms which do not vanish. Since it is the symmetry breaking properties that matter when constructing the effective chiral Lagrangian, the form of the latter is the same whether or not the vanishing terms are kept. Nevertheless, we drop these terms as it simplifies the equations.

down to its hypercubic subgroup, but these only enter the chiral Lagrangian at $O(a^2m^2)$ because of the need to have four derivatives.

The analysis of fermionic operators in the untwisted Wilson theory has been carried out in Refs. [27,28]. There are fermion bilinears and four-fermion operators. What is found, however, is that the only operators which break more symmetries than those already broken by $\mathcal{L}_0 + \mathcal{L}_1$ are the bilinears which break rotation symmetry down to its hypercubic subgroup. As for the gluonic operators discussed above, these contribute beyond quadratic order in our expansion. The contributions of the remaining operators to the effective chiral Lagrangian are of exactly the same form as those obtained by treating the effects at $\mathcal{L}_1$ at second-order. Thus we do not list these operators.

This leaves the new dimension six operators induced by the twisted mass. These, however, are all of cubic or higher order in our expansion. This is because they have at least one factor of μ in addition to the a^2 common to all operators in $\mathcal{L}_2$. An important example is the twisted Pauli term discussed above.

Thus we conclude that, for the purpose of constructing the effective chiral Lagrangian to next-to-leading order (NLO) we need only keep the following terms at the quark level

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_g + \bar{\psi}(\slashed{D} + m + i\gamma_5\tau_3\mu)\psi + b_1 a\bar{\psi}i\sigma_{\mu\nu}F_{\mu\nu}\psi,$$
(11)

with the relations to bare parameters given in Eqs. (6), (7) and (8). The only difference from the result for the standard Wilson theory given in Ref. [7] is the addition of a twisted mass term.

C. Effective chiral Lagrangian

Following [7], the next step is to write down a generalization of the continuum chiral Lagrangian that includes the effects of the Pauli term. As already noted, we use the following power-counting scheme[4]:

$$1 \gg \{\mathsf{m}, p^2, a\} \gg \{\mathsf{m}^2, \mathsf{m}p^2, p^4, a\mathsf{m}, ap^2, a^2\}$$
$$\gg \{\mathsf{m}^3, \ldots\}.$$
(12)

Here m is a generic mass parameter that can be either the renormalized normal mass m, or the renormalized twisted mass μ. There is no O(1) term in the chiral expansion for pions. The leading order (LO) terms are of linear order in this expansion, and the NLO terms of quadratic order. We work to NLO, which is sufficient for the study of the phase diagram. We stress that we can use the expansion in other regimes, e.g., $\mathsf{m} \gg a$ or $\mathsf{m} \sim a^2$, except that we then need to drop certain terms which become of too high order.

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[4]Factors of Λ needed to make quantities dimensionless are implicit from now on unless otherwise specified

The chiral Lagrangian is built from the SU(2) matrix-valued Σ field, which contains the relevant low-energy degrees of freedom. It transforms under the chiral group $SU(2)_L \times SU(2)_R$ as

$$\Sigma \rightarrow L\Sigma R^\dagger, \qquad L \in SU(2)_L, \qquad R \in SU(2)_R. \quad (13)$$

The vacuum expectation value of Σ_0 breaks the chiral symmetry down to an SU(2) subgroup. The fluctuations around Σ_0 correspond to the pseudoscalar mesons (pions):

$$\Sigma(x) = \Sigma_0 \exp\left\{i\sum_{a=1}^{3}\pi_a(x)\tau_a/f\right\}$$
$$= \Sigma_0\{\cos[\pi(x)/f] + i\hat{\boldsymbol{\pi}}(x)\cdot\boldsymbol{\tau}\sin[\pi(x)/f]\}, \quad (14)$$

where f is the decay constant (normalized so that $f_\pi = 93$ MeV). The norm and the unit vector of the pion fields are given by $\pi = \sqrt{\boldsymbol{\pi}\cdot\boldsymbol{\pi}} = \pi_a\pi^a$ and $\hat{\pi}_a = \pi_a/\pi$.

The chiral Lagrangian can be obtained from the quark Lagrangian, Eq. (11), by a standard spurion analysis. We must introduce a spurion matrix $\hat{A}$ for the Pauli term, as well as the usual spurion χ for the mass terms. Both transform in the same way as the Σ field. At the end of the analysis the spurions are set to their respective constant values

$$\chi \longrightarrow 2B_0(m + i\tau^3\mu) \equiv \hat{m} + i\tau^3\hat{\mu},$$
$$\hat{A} \longrightarrow 2W_0 a \equiv \hat{a},$$
(15)

where B_0 and W_0 are unknown dimensionful parameters, and we have defined useful quantities $\hat{m}$, $\hat{\mu}$ and $\hat{a}$. Note that the only change caused by the presence of the twisted mass is the appearance of the μ term in the constant value of χ. Other than this, the construction of the chiral Lagrangian is identical to that for untwisted Wilson fermions.

Because of this simplification, we can read off the form of the chiral Lagrangian for tmLQCD from Ref. [28], in which the Lagrangian for untwisted Wilson fermions was worked out to quadratic order in our expansion. The only extension we make is to include sources for currents and densities. The left- and right-handed currents are introduced in the standard way by using the covariant derivative $D_\mu\Sigma = \partial_\mu\Sigma - il_\mu\Sigma + i\Sigma r_\mu$, and the associated field strengths, e.g., $L_{\mu\nu} = \partial_\mu l_\nu - \partial_\nu l_\mu + i[l_\mu, l_\nu]$, and enforcing invariance under local chiral transformations [29,30]. Sources for scalar and pseudoscalar densities are similarly included if we write $\chi = 2B_0(s + ip)$, with s and p hermitian matrix fields. Although the sources play no role in the discussion of the phase diagram, we have used them to obtain forms for various matrix elements of phenomenological interest [15]. These results will be described elsewhere [16].

Putting these ingredients together the resulting effective chiral Lagrangian is (in Euclidean space)

$$
\begin{aligned}
\mathcal{L}_\chi = {} & \frac{f^2}{4}\mathrm{Tr}(D_\mu\Sigma D_\mu\Sigma^\dagger) - \frac{f^2}{4}\mathrm{Tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi) - \frac{f^2}{4}\mathrm{Tr}(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A}) - L_1\mathrm{Tr}(D_\mu\Sigma D_\mu\Sigma^\dagger)^2 \\
& - L_2\mathrm{Tr}(D_\mu\Sigma D_\nu\Sigma^\dagger)\mathrm{Tr}(D_\mu\Sigma D_\nu\Sigma^\dagger) + (L_4 + L_5/2)\mathrm{Tr}(D_\mu\Sigma^\dagger D_\mu\Sigma)\mathrm{Tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi) + L_5\{\mathrm{Tr}[(D_\mu\Sigma^\dagger D_\mu\Sigma) \\
& \times (\chi^\dagger\Sigma + \Sigma^\dagger\chi)] - \mathrm{Tr}(D_\mu\Sigma^\dagger D_\mu\Sigma)\mathrm{Tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)/2\} - (L_6 + L_8/2)[\mathrm{Tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)]^2 \\
& - L_8\{\mathrm{Tr}[(\chi^\dagger\Sigma + \Sigma^\dagger\chi)^2] - [\mathrm{Tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)]^2/2\} - L_7[\mathrm{Tr}(\chi^\dagger\Sigma - \Sigma^\dagger\chi)]^2 + iL_{12}\mathrm{Tr}(L_{\mu\nu}D_\mu\Sigma D_\nu\Sigma^\dagger \\
& + R_{\mu\nu}D_\mu\Sigma^\dagger D_\nu\Sigma) + L_{13}\mathrm{Tr}(L_{\mu\nu}\Sigma R_{\mu\nu}\Sigma) + (W_4 + W_5/2)\mathrm{Tr}(D_\mu\Sigma^\dagger D_\mu\Sigma)\mathrm{Tr}(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A}) \\
& - (W_6 + W_8/2)\mathrm{Tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)\mathrm{Tr}(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A}) + W_{10}\mathrm{Tr}(D_\mu\hat{A}^\dagger D_\mu\Sigma + D_\mu\Sigma^\dagger D_\mu\hat{A}) \\
& - (W_6' + W_8'/2)[\mathrm{Tr}(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A})]^2 \\
& + \text{contact terms}.
\end{aligned}
\tag{16}
$$

Here the L_i's are the standard Gasser-Leutwyler low-energy constants of continuum chiral perturbation theory, and the W_i's and W_i''s unknown low-energy constants associated with discretization errors. For the latter constants we use the notation of Ref. [28,31]. In fact, these constants related to discretization are the same as those for the untwisted Wilson theory, assuming the same gauge action, since the twisting enters only through the parameters in the spurions.

In writing (16) we have used various simplifications that result from the fact that the flavor group is SU(2). In particular, because $\hat{A}$ is, in the end, proportional to an element of SU(2) with a real proportionality constant, and because we do not use it as a source, we can take $\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A}$ to be proportional to the identity matrix, and $\mathrm{Tr}(\hat{A}^\dagger\Sigma - \Sigma^\dagger\hat{A})$ to vanish. Thus the following possible terms vanish for SU(2):

$$
\begin{aligned}
& + W_5\{\mathrm{Tr}[(D_\mu\Sigma^\dagger D_\mu\Sigma)(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A})] - \mathrm{Tr}(D_\mu\Sigma^\dagger D_\mu\Sigma)\mathrm{Tr}(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A})/2\} - W_8\{\mathrm{Tr}[(\chi^\dagger\Sigma + \Sigma^\dagger\chi)(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A})] \\
& - \mathrm{Tr}(\chi^\dagger\Sigma + \Sigma^\dagger\chi)\mathrm{Tr}(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A})/2\} - W_7\mathrm{Tr}(\chi^\dagger\Sigma - \Sigma^\dagger\chi)\mathrm{Tr}(\hat{A}^\dagger\Sigma - \Sigma^\dagger\hat{A}) - W_8'\{\mathrm{Tr}[(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A})^2] \\
& - [\mathrm{Tr}(\hat{A}^\dagger\Sigma + \Sigma^\dagger\hat{A})]^2/2\} - W_7'[\mathrm{Tr}(\hat{A}^\dagger\Sigma - \Sigma^\dagger\hat{A})]^2.
\end{aligned}
\tag{17}
$$

Similarly, the operators multiplied by L_5, L_7 and L_8 alone in (16) do not contribute once we set χ to $2B_0(m + i\tau^3\mu)$, although they are needed when using χ as a source. They do not contribute in our subsequent study of the phase diagram.

Finally, we comment on the W_{10} term, which is present only because we include both discretization errors and external sources. This term can, in fact, be removed using the equations of motion, but we have found that it provides a useful diagnostic in computations of matrix elements.

Our result (16) agrees with, and extends, the work of Ref. [8], in which the chiral Lagrangian for tmLQCD including effects linear in a was determined. Our generalizations are to include the term of O(a^2), to make the simplifications due to using the group SU(2), and to include the sources for currents. In comparing our result to that in Ref. [8] it should be noted that the result in that work is expressed in the physical basis, while we use the twisted basis. The two results are related by a nonanomalous axial rotation.

III. ANALYSIS OF PHASE DIAGRAM

To investigate the phase diagram of tmLQCD, we are interested in the vacuum state of the effective continuum chiral theory. To the order that we are working, the potential energy is

$$
\begin{aligned}
V_\chi = {} & -\frac{c_1}{4}\mathrm{Tr}(\Sigma + \Sigma^\dagger) + \frac{c_2}{16}[\mathrm{Tr}(\Sigma + \Sigma^\dagger)]^2 \\
& + \frac{c_3}{4}\mathrm{Tr}[i(\Sigma - \Sigma^\dagger)\tau_3] + \frac{c_4}{16}\{\mathrm{Tr}[i(\Sigma - \Sigma^\dagger)\tau_3]\}^2 \\
& + \frac{c_5}{16}\mathrm{Tr}[i(\Sigma - \Sigma^\dagger)\tau_3]\mathrm{Tr}(\Sigma + \Sigma^\dagger),
\end{aligned}
\tag{18}
$$

where the explicit forms of the coefficients, and their sizes in our power-counting scheme, are

$$
\begin{aligned}
& c_1 = f^2(\hat{m} + \hat{a}) \sim m + a, \qquad c_2 = -8[(2L_6 + L_8)\hat{m}^2 + (2W_6 + W_8)\hat{a}\,\hat{m} + (2W_6' + W_8')\hat{a}^2] \sim m^2 + am + a^2, \\
& c_3 = f^2\hat{\mu} \sim \mu, \qquad c_4 = -8(2L_6 + L_8)\hat{\mu}^2 \sim \mu^2, \qquad c_5 = 16[(2L_6 + L_8)\hat{m}\,\hat{\mu} + (W_6 + W_8/2)\hat{a}\,\hat{\mu}] \sim \mu(m + a).
\end{aligned}
\tag{19}
$$

Note that there are no relations between the c_i coefficients: all five are independent at nonzero lattice spacing. The extra terms introduced by twisting are those with coefficients c_3, c_4 and c_5.

To determine the pattern of symmetry breaking as a function of the coefficients c_i, we repeat the analysis of [7]. We distinguish three regions of quark masses, each successively smaller by a factor of a:

(i) **Physical quark masses:** $1 \gg m \sim \mu \gg a$. In this case, both discretization errors and terms of quadratic order in masses can be neglected, so that only the $c_1 \sim m$ and $c_3 \sim \mu$ terms need be kept. In this case the symmetry breaking is as in the continuum. In particular, the condensate Σ_0 lies in the direction of the full mass term, so that:

$$\Sigma_0 = \frac{(m + i\tau_3\mu)}{\sqrt{m^2 + \mu^2}} = \frac{(\hat{m} + i\tau_3\hat{\mu})}{\sqrt{\hat{m}^2 + \hat{\mu}^2}}. \qquad (20)$$

The pions are degenerate, with masses

$$m_\pi^2 = \sqrt{\hat{m}^2 + \hat{\mu}^2}[1 + O(a, m, \mu)]. \qquad (21)$$

Note that this result holds also if either $m \gg a$ or $\mu \gg a$.

(ii) **Significant discretization errors:** $1 \gg m \sim \mu \sim a$. This is the parameter region for which our expansion is most natural. The LO coefficients $c_{1,3}$ still dominate over the NLO coefficients $c_{2,4,5}$, but the $O(a)$ term in c_1 cannot be ignored. Thus the results for region (i) still hold, except that the untwisted quark mass $\hat{m}$ must be replaced by the shifted mass $\hat{m}' = \hat{m} + \hat{a}$, or equivalently $m \to m' = m + aW_0/B_0$. In other words, there is an $O(a)$ shift in the critical mass, as noted in Ref. [7]. In terms of this new mass the coefficients become

$$c_1 \sim m', \qquad c_2 \sim m'^2 + am' + a^2, \qquad c_3 \sim \mu,$$
$$c_4 \sim \mu^2, \qquad c_5 \sim \mu(m' + a). \qquad (22)$$

(iii) **Aoki region:** $m' \sim \mu \sim a^2$. In this region the nominally NLO coefficient c_2 is of the same size as the LO coefficients $c_{1,3}$; all are of $O(a^2)$. The other NLO coefficients remain suppressed by at least one power of a: $c_4 \sim a^4$, $c_5 \sim a^3$. The fact that LO and some NLO coefficients are comparable might suggest a breakdown in convergence. This is not so, however. The largest NNLO term in this parameter region is $\sim a^3$, and thus suppressed by one power of a. Loop corrections are also suppressed, since they are quadratic in m' and μ (up to logarithms) and thus $\sim a^4$. The key result that allows this reordering of the series is that the leading order discretization error has exactly the same form as the term proportional to m and so can be completely absorbed into m', to all orders in the chiral expansion.

As in the untwisted Wilson theory, it is the competition between the LO terms and the NLO c_2 term that can lead to interesting phase structure. Note that *both* m' and μ must be of $O(a^2)$ in order for such competition to occur; if either m' or μ is of $O(a)$ then one is in the continuumlike region (ii).

To determine the condensate we must minimize the potential energy (18). We parameterize the chiral field in the standard way: $\Sigma = A + i\mathbf{B} \cdot \boldsymbol{\tau}$ with real A and $\mathbf{B}$ satisfying $A^2 + \mathbf{B}^2 = 1$, so that $A, B_i \in [-1, 1]$. Similarly, the condensate (the value of Σ that minimizes the potential) is written $\Sigma_0 = A_m + i\mathbf{B}_m \cdot \boldsymbol{\tau}$. In the Aoki region the potential is[5]

$$V_\chi = -c_1 A - c_3 B_3 + c_2 A^2. \qquad (23)$$

Although $c_1 = f^2\hat{m}'$ and $c_3 = f^2\hat{\mu}$ can both take either sign, we need only consider the case when both are positive. The other possibilities can be obtained using the symmetries of V_χ: if $c_1 \to -c_1$ with $c_{2,3}$ fixed (i.e., when $m' \to -m'$), the condensate changes as $A_m \to -A_m$, $B_{3,m} \to B_{3,m}$; while if $c_3 \to -c_3$ with $c_{1,2}$ fixed (i.e., when $\mu \to -\mu$), then $A_m \to A_m$, $B_{3,m} \to -B_{3,m}$. We do not need to specify the transformation of the other two components of the condensate since they vanish, as we now show.

To do so it is useful to define r and θ by

$$A = r\cos\theta, \qquad B_3 = r\sin\theta, \qquad A^2 + B_3^2 = r^2,$$
$$B_1^2 + B_2^2 = 1 - r^2, \qquad 0 \le r \le 1, \qquad (24)$$

in terms of which the potential becomes

$$V_\chi = -r(c_1\cos\theta + c_3\sin\theta) + r^2 c_2\cos^2\theta. \qquad (25)$$

We will first minimize this at fixed r, and then minimize with respect to r. Based on the symmetries just discussed, we consider only $c_{1,3} > 0$. At fixed r, the term linear in r, $-(c_1\cos\theta + c_3\sin\theta)$, has its minimum in the quadrant $0 < \theta < \pi/2$, while the term quadratic in r, $c_2\cos^2\theta$, has its minima at $\pm\pi/2$ for $c_2 > 0$ and $0, \pi$ for $c_2 < 0$. It follows that, irrespective of the sign of c_2, the minimizing angle, $\theta_0(r)$, also lies in the first quadrant: $0 < \theta_0(r) < \pi/2$. Its actual value is given by the appropriate solution to

$$c_1\sin\theta_0(r) - c_3\cos\theta_0(r) = c_2 r\sin[2\theta_0(r)], \qquad (26)$$

and we denote the value of the potential at the minimum by $V_{\chi,\min}(r)$. To minimize with respect to r we evaluate the derivative:

$$\frac{dV_{\chi,\min}(r)}{dr} = \frac{\partial V_\chi}{\partial r}\Big|_{\theta=\theta_0(r)} = -\frac{c_3}{\sin\theta_0(r)}, \qquad (27)$$

where to obtain this simple form we have used Eq. (26). Since $c_3 > 0$ by assumption, and $\sin\theta_0(r) > 0$ as $\theta_0(r)$ lies in the first quadrant, we find that $V_{\chi,\min}(r)$ is a monotoni-

---

[5]Henceforth, we will drop references to the $O(a^3)$ corrections.

cally decreasing function of r. The symmetries discussed above show that this holds for any $c_{1,3}$. Thus the absolute minimum of V_χ is at $r = 1$, and the minimizing angle is $\theta_m \equiv \theta_0(r = 1)$.

At this point it is useful to introduce scaled variables

$$\alpha = \frac{c_1}{|c_2|} = \frac{f^2(\hat{m} + \hat{a})}{8|2W_6' + W_8'|\hat{a}^2} \sim m'/a^2, \quad (28)$$

$$\beta = \frac{c_3}{|c_2|} = \frac{f^2\hat{\mu}}{8|2W_6' + W_8'|\hat{a}^2} \sim \mu/a^2. \quad (29)$$

In words, α is the shifted, untwisted mass in units proportional to a^2, while β is the twisted mass in the same units. In the Aoki region α and β are of order unity. In terms of these variables, the equation to be solved to determine $A_m = \cos\theta_m$ is

$$A_m^4 \mp \alpha A_m^3 + \frac{\alpha^2 + \beta^2 - 4}{4}A_m^2 \pm \alpha A_m - \frac{\alpha^2}{4} = 0. \quad (30)$$

[This is just Eq. (26) for $r = 1$ after some manipulation.] Here the upper sign is for $c_2 > 0$, the lower for $c_2 < 0$. One must pick solutions with A_m real and satisfying $-1 \leq A_m \leq 1$, and of these choose that which minimizes V_χ. Given A_m, the other components are given by

$$B_{1,m} = B_{2,m} = 0, \qquad B_{3,m} = \text{sign}(c_3)\sqrt{1 - A_m^2}, \quad (31)$$

where the sign of $B_{3,m}$ follows from the form of the potential, Eq. (23).

The pion masses are given by the quadratic fluctuations about the condensate, using Eq. (14). The unbroken U(1) flavor symmetry ensures that the charged pions are degenerate. We find

$$m_{\pi_1}^2 = m_{\pi_2}^2 = \frac{c_1 A_m + c_3 B_{3,m} - 2c_2 A_m^2}{f^2} = \frac{|c_2|}{f^2}\frac{\beta}{B_{3,m}}, \quad (32)$$

$$\Delta m_\pi^2 \equiv m_{\pi_3}^2 - m_{\pi_1}^2 = \frac{2c_2 B_{3,m}^2}{f^2}, \quad (33)$$

where to obtain the final form for charged pions we have used Eq. (26). It is straightforward to show that none of the pion masses become negative for any values of the parameters.

Before we show plots of the results, it is useful to discuss how the sign of c_2 affects the solutions. Recall that the sign of c_2 depends on the gauge action, and is not known *a priori*. For the untwisted Wilson action, the sign has an important impact: the Aoki phase appears only for $c_2 > 0$, while there is a first order transition for $c_2 < 0$. Once we extend the theory into the full twisted mass plane, however, the two possibilities are related. We focus on the $A - B_3$ plane (i.e., we set $r = 1$) since we know from above that the minimum of the potential lies in this

plane for all c_2. The potential in this plane is

$$V_\chi = -c_1\cos\theta - c_3\sin\theta + c_2\cos^2\theta. \quad (34)$$

If we change variables as follows

$$c_1 = c_3', \qquad c_3 = -c_1', \qquad c_2 = -c_2', \\ \theta = \theta' - \pi/2, \quad (35)$$

so that $\cos\theta = \sin\theta'$ and $\sin\theta = -\cos\theta'$, then the potential has the same form

$$V_\chi = -c_1'\cos\theta' - c_3'\sin\theta' + c_2'\cos^2\theta' - c_2', \quad (36)$$

aside from an overall shift. This implies that if we take the phase diagram for, say $c_2 > 0$, and rotate it anticlockwise by 90°, we will obtain the phase diagram for $c_2' = -c_2 < 0$, with the components of the condensate given by $A_m' = -B_{3,m}$ and $B_{3,m}' = A_m$. The mass of π_3 is given simply by its value at the rotated point, $m_{\pi_3}' = m_{\pi_3}$.

This discussion does not include fluctuations in the other two directions. To obtain the charged pion masses, however, we can use the general result Eq. (33) for the splitting between charged and neutral pion masses, and the equality of the neutral masses, to obtain

$$(m_{\pi_1}')^2 = m_{\pi_1}^2 + \Delta m_\pi^2 - \Delta m_\pi'^2 \quad (37)$$

$$= m_{\pi_1}^2 + \frac{2c_2\sin^2\theta_m}{f^2} - \frac{2c_2'\sin^2\theta_m'}{f^2} \quad (38)$$

$$= m_{\pi_1}^2 + \frac{-2c_2'\cos^2\theta_m'}{f^2} - \frac{2c_2'\sin^2\theta_m'}{f^2} \quad (39)$$

$$= m_{\pi_1}^2 - \frac{2c_2'}{f^2}. \quad (40)$$

Thus we find a fixed offset (independent of c_1 and c_3) between the charged pion masses. The offset has the correct sign so that all pions have positive or zero mass-squared. In particular, if $c_2 > 0$ there is an Aoki phase with $m_{\pi_1} = 0$. This rotates (as shown in Fig. 1(b)] into a phase with $m_{\pi_1}'^2 = -2c_2'/f^2 = +2c_2/f^2 > 0$.

It is straightforward to solve the quartic equation and determine the condensate and pion masses. The only subtlety is that care must be taken when either β or α is set to zero. This can be seen, for example, from the final form for the charged pion masses, Eq. (32), which becomes $0/0$ when $\beta \to 0$. In either of these two limits, $\alpha \to 0$ or $\beta \to 0$, the quartic equation reduces to a quadratic. The solutions for $\beta \to 0$ have been given in Ref. [7], and we do not repeat them here. Those for $\alpha \to 0$ can be obtained from those for $\beta \to 0$ using the 90° rotation in the mass plane just discussed.

For the remainder of this article we illustrate the nature of the phase diagram by plotting the condensate and pion

masses. We display results as a function of α for fixed β and c_2. We only show results for $\beta \geq 0$ since, as explained above, those for $\beta < 0$ differ only by changing the sign of $B_{3,m}$. In particular, the pion masses are symmetrical under $\beta \rightarrow -\beta$. We could also consider only $\alpha \geq 0$, but find it clearer to show results for both signs.

We begin with results for $c_2 > 0$. Figure 2 shows the form of the identity component of the condensate, $A_m = \mathrm{Tr}(\Sigma_0)/2$, for $\beta = 0, 1, 2$ and 3. The corresponding pion masses are shown in Fig. 3. In the untwisted theory ($\beta = 0$) there are second order transitions at $\alpha = \pm 2$, as shown by the kinks in A_m and the vanishing of the pion masses. The Aoki phase, with $B_{3,m} \neq 0$, which breaks flavor and parity, and correspondingly has two Goldstone bosons, lies between these second order points. Once β is nonvanishing, however, the transition is smoothed out into a crossover, and the pion masses are always nonzero. Flavor is broken for all α, with the charged pions heavier than the neutral pion by $O(a^2)$, as given by Eq. (33). For the special case of $\alpha = 0$ (maximal twisting), A_m vanishes and $B_{3,m}^2 = 1$, so the mass-squared splitting is $2c_2/f^2$ for all β (which becomes a difference of 2 in the units in the plots).

It is now possible to pass through the Aoki phase by varying β, i.e., by changing the sign of the twisted mass. When doing so there is a first order phase transition, since $B_{3,m}$ jumps from $+\sqrt{1 - A_m^2} = \sqrt{1 - \alpha^2/4}$ to $-\sqrt{1 - A_m^2} = -\sqrt{1 - \alpha^2/4}$.

We now consider the case where c_2 is negative. Figure 4 shows A_m and the pion masses as a function of α for fixed values of β. Figure 4(a) and Fig. 4(b) show the results for $\mu = 0$. As discussed in Ref. [7], the condensate jumps from $\Sigma_0 = 1$ (and thus $A_m = 1$, $\mathbf{B} = 0$) for $\alpha > 0$ to $\Sigma_0 = -1$ (and thus $A_m = -1$, $\mathbf{B} = 0$) for $\alpha < 0$. This is a first order transition without flavor breaking, so all pions remain massive and degenerate.
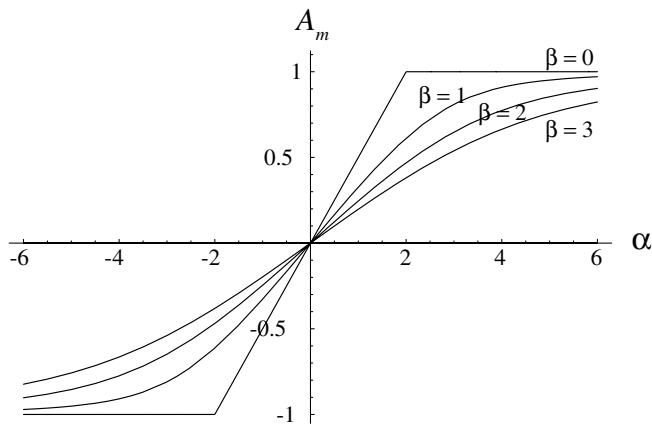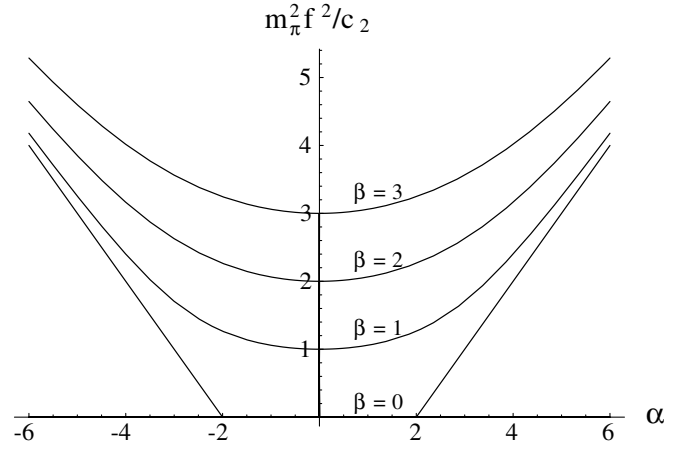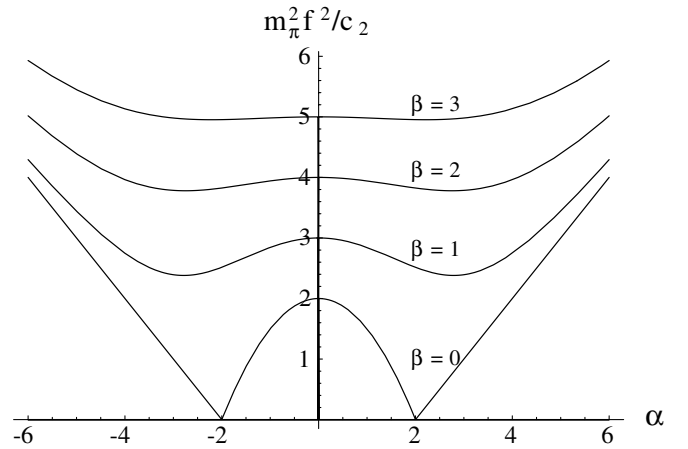

(a) Mass of π_1 and π_2

(b) Mass of π_3

FIG. 3.   Mass of the pions as a function of α, for $c_2 > 0$ and $\beta = 0, 1, 2, 3$.

FIG. 2.   The global minimum of the potential, A_m, as a function of α, for $c_2 > 0$ and $\beta = 0, 1, 2, 3$.

The remainder of Fig. 4 shows what happens at nonzero twisted mass. The effect of μ is to twist the condensate, so that there is a nonzero τ_3 component $B_{3,m}$. There is, however, still a first order transition at which $B_{3,m}$ flips sign between $\pm(1 - \beta/2)$ (assuming $\beta > 0$). The neutral pion is now lighter than the charged pions due to the explicit flavor breaking. The neutral pion has a mass $m_{\pi_3}^2 = 2|c_2|(1 - \beta/2)^2/f^2$ at the transition, while, as noted above, the charged pions have a constant mass given by $m_{\pi_{1,2}}^2 = 2|c_2|/f^2$. The transition weakens as $|\beta|$ increases, and ends with a second order transition point at $\beta = \pm 2$, at which the neutral pion is massless [see Fig. 4(f)]. For larger β the transition is smoothed out. Note that, once away from the transition, for $\alpha = 0$ the mass-squared splitting between charged and neutral pions is $2|c_2|/f^2$.
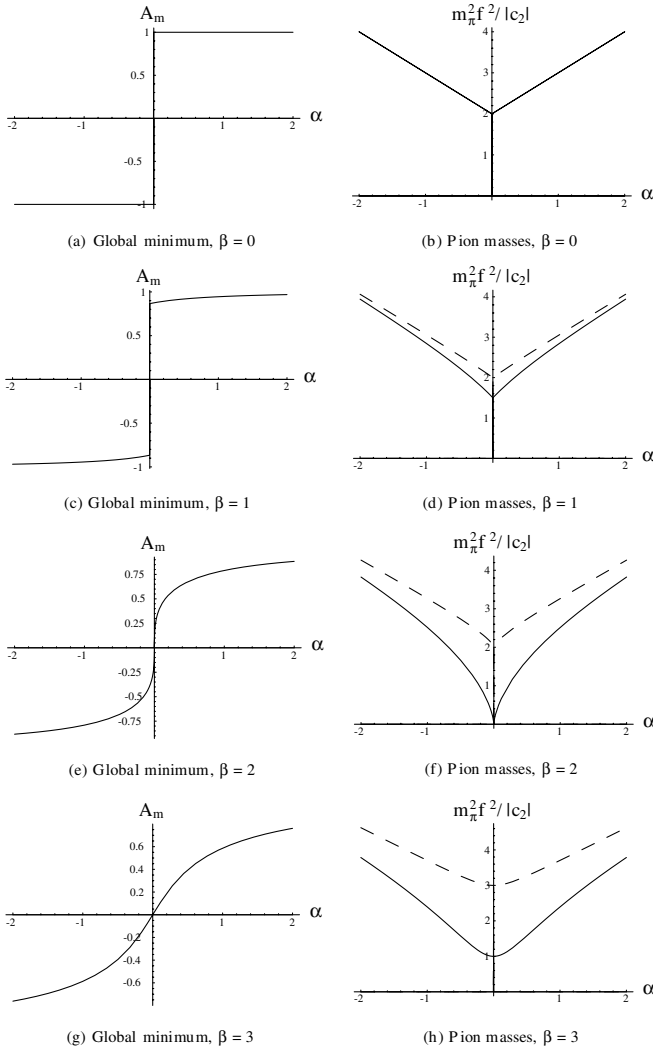
FIG. 4. Global minimum A_m [(a), (c), (e), (g)] and pion masses [(b), (d), (f), (h)] as a function of α, for $c_2 < 0$ and $\beta = 0, 1, 2, 3$. The dashed lines are for $\pi_{1,2}$ and the solid lines are for π_3.

(a) Mass of π_1 and π_2

(b) Mass of π_3

FIG. 5. Mass of the pions as a function of β, for $c_2 < 0$ and $\alpha = 0, 1, 2, 3$.

These plots illustrate the general result shown above, namely, that the $c_2 < 0$ case can be obtained from that with $c_2 > 0$ by a 90° rotation and appropriate redefinitions. Indeed, the results for $c_2 > 0$ can alternatively be viewed as the plots for $c_2 < 0$ at fixed α with β varying, and *vice versa*, with the exception of the charged pion masses, which differ by a constant offset of $2|c_2|/f^2$. To illustrate this latter point we plot, in Fig. 5, the pion masses for $c_2 < 0$ as a function of β for fixed values of $\alp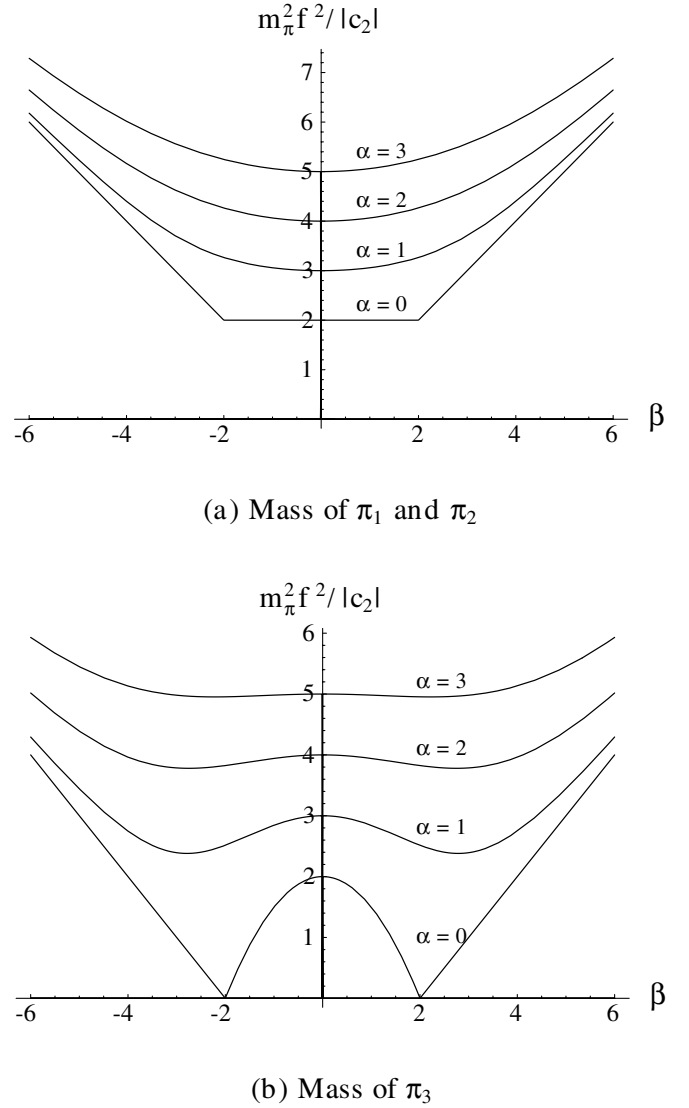ha$. Comparing to Fig. 3, we see the equality of the neutral pion masses and the constant offset in the charged pion masses.

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