

**Quarks with twisted boundary conditions in the epsilon regime**Thomas Mehen<sup>1,2,3,\*</sup> and Brian C. Tiburzi<sup>1,3,†</sup><sup>1</sup>*Department of Physics, Duke University, Durham, North Carolina 27708, USA*<sup>2</sup>*Jefferson Laboratory, 12000 Jefferson Avenue, Newport News, Virginia 23606, USA*<sup>3</sup>*Institute for Nuclear Theory, University of Washington, Seattle, Washington 98195, USA*

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We study the effects of twisted boundary conditions on the quark fields in the epsilon regime of chiral perturbation theory. We consider the  $SU(2)_L \times SU(2)_R$  chiral theory with nondegenerate quarks and the  $SU(3)_L \times SU(3)_R$  chiral theory with massless up and down quarks and massive strange quarks. The partition function and condensate are derived for each theory. Because flavor-neutral Goldstone bosons are unaffected by twisted boundary conditions chiral symmetry is still restored in finite volumes. The dependence of the condensate on the twisting parameters can be used to extract the pion decay constant from simulations in the epsilon regime. The relative contribution to the partition function from sectors of different topological charge is numerically insensitive to twisted boundary conditions.

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**I. INTRODUCTION**

Understanding the strongly interacting regime of quantum chromodynamics (QCD) remains a challenging problem in physics. The dynamics is nonperturbative and results in the confinement of the colored quark and gluon degrees of freedom. Numerically simulating the gauge theory on a spacetime lattice provides a first principles method for determining the properties of the color neutral hadrons that are observed in nature. Recently, there has been much effort in applying effective field theory methods to quantitatively compute the effect of lattice artifacts such as unphysical quark masses, quenching, finite lattice spacing, and finite volume on lattice simulations of hadronic observables. Effective field theory calculations can be used to extrapolate the results of simulations with unphysical parameters to real world observables [1]. One also can use the dependence on lattice artifacts to extract the parameters appearing in low-energy effective Lagrangians of QCD.

Lattice QCD simulations usually employ periodic boundary conditions for the quark and gluon fields. The results of a simulation should be independent of the choice of boundary conditions as one takes the volume to infinity, so there is considerable freedom in choosing the boundary conditions for the fields. However, the action must be single valued so that observables are well defined. Fields need only be periodic up to a transformation which is symmetry of the action. If a generic field  $\phi$  depends on a lattice coordinate  $x_i$  which is defined on the interval  $0 < x_i < L$ , then we must have

$$\phi(x_i + L) = U\phi(x_i),$$

where  $U$  is a symmetry of the action and  $U^\dagger U = 1$ . When  $U \neq 1$ , these are called twisted boundary conditions. This is equivalent to gauging a global symmetry of the action

and then turning on a uniform background gauge field. In infinite space, a constant background gauge field can be removed by a gauge transformation, so there are no physical consequences in the infinite volume limit. However, a uniform background gauge field can modify the physics of a compact space. Different applications of twisted boundary conditions have appeared throughout the years [2–11].<sup>1</sup> Recently, there has been a renewed interest in twisted boundary conditions in lattice QCD simulations [20–24]. This recent work has focused on using twisted boundary conditions on quarks as a means of avoiding the restriction of lattice momenta to integer multiples of  $2\pi/L$ .

In this paper, we consider a different aspect of twisted boundary conditions. Since dynamical effects due to twisting show up as corrections at finite volume, it is natural to examine the effects of twisted boundary conditions in the  $\epsilon$  regime of chiral perturbation theory ( $\chi$ PT), where volume effects are non-negligible.  $\chi$ PT is the low-energy effective theory of QCD that encodes the dynamics of pseudo-Goldstone bosons that emerge from spontaneous breaking of chiral symmetry. Spontaneous symmetry breaking does not occur in finite volume. Therefore the perturbative expansion of  $\chi$ PT must breakdown in the limit  $m_q \rightarrow 0$  with  $L$  held constant. Indeed when  $m_\pi L \ll 1$  the zero momentum mode of the Goldstone boson becomes strongly coupled. In this limit, the path integral over the zero modes must be treated exactly, while nonzero modes can be treated perturbatively. Computation of the chiral symmetry breaking order parameter in this regime shows that the chiral condensate vanishes exponentially as  $m_\pi^2 f_\pi^2 \beta V \rightarrow 0$ , where  $\beta V$  is the four-dimensional volume of the lattice. For early references on these finite-size effects in theories with spontaneously broken symmetries,

\*Electronic address: mehen@phy.duke.edu

†Electronic address: bctiburzi@phy.duke.edu

<sup>1</sup>The use of twisted boundary conditions in the time direction can be utilized to produce an imaginary chemical potential [12–19].

see [25–31]. For later investigations and numerical simulations see, for example, [32–41].

In the  $p$  regime of chiral perturbation theory one takes  $1/L \sim m_\pi \sim Q$  so propagators scale as  $Q^{-2}$ , vertices scale as  $Q^2$  or higher (since vertices have at least two derivatives or one insertion of the quark mass) and loop integrations (or sums in finite volume) scale as  $Q^4$ . The contribution to the partition function from an arbitrary vacuum graph scales as  $Q^n$  where  $n \geq 4l - 2I + 2V = 2l + 2$ ,  $l$  is the number of loops,  $I$  is the number of internal lines, and  $V$  is the number of vertices. Thus, in this regime the partition function can be computed in perturbation theory. In the  $\varepsilon$  regime,  $1/L \sim \varepsilon$  but  $m_\pi \sim \varepsilon^2$ . Thus, the zero momentum mode is singled out because its propagator scales as  $\varepsilon^{-4}$  while the nonzero mode propagators scale as  $\varepsilon^{-2}$ . The leading order interactions of zero modes with themselves are proportional to  $m_\pi^2 \sim \varepsilon^4$  so an arbitrary vacuum graph with only zero momentum modes and leading order vertices scales as  $\varepsilon^{4l - 4I + 4V} = \varepsilon^4$ . Therefore, an infinite number of graphs with zero momentum modes must be resummed at leading order. This resummation is straightforward because the theory of zero modes alone is simply a matrix integral.

Now we see how this power counting is modified in the presence of twisted boundary conditions. The twisted boundary conditions induce a constant shift in the momentum of the propagators of fields that are charged under the background gauge field:

$$\frac{1}{k_\mu^2 + m_\pi^2} \rightarrow \frac{1}{(k_\mu + B_\mu)^2 + m_\pi^2}, \quad (1)$$

where  $B_\mu$  is the background gauge field. For generic twists,  $B_\mu \sim 1/L \sim \varepsilon$  and the propagator in Eq. (1) scales as  $\varepsilon^{-2}$ . The zero modes of fields charged under the background gauge field are no longer strongly coupled. However, if there are Goldstone bosons that are not charged under the background gauge field their zero modes will continue to be strongly coupled. In QCD with  $N$  quarks,  $B_\mu$  must couple either to baryon number [20], in which case all meson fields are neutral, or an element of the  $SU(N)$  flavor group. Because quark mass differences and electric charge break the flavor symmetry down to the diagonal subgroup, we will only consider twists that are flavor diagonal. Then the flavor-neutral Goldstone bosons will be neutral under the background field and there still will be a restoration of chiral symmetry as  $m_q \rightarrow 0$  with  $L$  fixed.<sup>2</sup> The qualitative behavior of the condensate as a function of  $m_q$  is the same as without twisting. However, not all the zero modes of the coset  $SU(N)_L \times SU(N)_R / SU(N)_V$  are strongly coupled, only those valued in the diagonal subgroup. The behavior of the condensate is quantitatively different in this case.

<sup>2</sup>Even for generic twists it is easy to show that there will be  $N - 1$  Goldstone bosons neutral under the background gauge field.

For sufficiently small twists the background gauge field can be comparable in size to  $m_\pi^2$  and the appropriate power counting is  $B_\mu \sim m_\pi \sim \varepsilon^2$ . In this case the zero modes of all Goldstone bosons are strongly coupled. We will refer to the case of  $B_\mu \sim m_\pi \sim \varepsilon^2$  as the twisted  $\varepsilon$  regime and  $B_\mu \sim \varepsilon, m_\pi \sim \varepsilon^2$  as the remnant  $\varepsilon$  regime.

In the untwisted theory at lowest order in the  $\varepsilon$  expansion, the partition function depends only on the mass term in the chiral Lagrangian. Computation of the volume dependence of the chiral condensate can be used to extract  $m_q \langle \bar{q}q \rangle_\infty$ , where  $\langle \bar{q}q \rangle_\infty$  is the infinite volume condensate. In the presence of twisted boundary conditions, however, the kinetic term in the chiral Lagrangian gives a leading order contribution to the partition function. By computing the finite-volume condensate as a function of both volume and twist, it is in principle possible to extract both  $m_q \langle \bar{q}q \rangle_\infty$  and  $f_\pi$ , where  $f_\pi$  is the pion decay constant. This latter quantity is usually extracted from the late time behavior of the axial correlator. Thus, twisted boundary conditions give an alternative method by which one may extract  $f_\pi$  from simulations in the  $\varepsilon$  regime.

We also evaluate the projection of the partition function onto sectors with fixed topological charge by including a  $\theta$  term in the chiral Lagrangian and Fourier transforming with respect to the  $\theta$  parameter. This calculation can be done analytically for the untwisted theory [42]. We perform the calculation for the isospin symmetric  $SU(2)_L \times SU(2)_R$  chiral theory. Twisted boundary conditions do not dramatically change the results of Ref. [42]. In particular, the observation that the QCD partition function is dominated by the sector with zero topological charge when  $m_q \langle \bar{q}q \rangle_\infty \beta V < 1$  still holds in the presence of twisted boundary conditions.

The paper is organized as follows: in Sec. II, we describe in detail the twisted boundary conditions imposed on the quark fields in QCD with  $N$  quark flavors and the twisted finite-volume meson propagator. We write down a general formula for the partition function in the presence of twisted boundary conditions. In Secs. III and IV, we evaluate this partition function as well as the finite-volume condensate for twisted  $SU(2)_L \times SU(2)_R$  and  $SU(3)_L \times SU(3)_R$  chiral theories, respectively. We consider both the twisted  $\varepsilon$  regime and the remnant  $\varepsilon$  regime. In Sec. V, we compute the projection of the partition function of the  $SU(2)_L \times SU(2)_R$  chiral theory onto sectors of fixed topological charge. Section VI contains a brief summary and discussion of directions for future work.

## II. GENERALITIES

Let us consider lattice QCD gauge theory with  $N$  quark flavors. In a finite volume, the boundary conditions on the quark fields must be chosen so that action is single valued. Thus the generator of any flavor symmetry of the action can be used to specify the boundary conditions of the quark fields. In the  $i$ th spatial direction, we impose flavor-

diagonal twisted boundary conditions of the form

$$q(x_i + L) = e^{i\Theta_i} q(x_i), \quad (2)$$

where the Abelian phases  $\Theta_\mu$  can be expanded in the Cartan subalgebra of  $U(N)$ . Instead of using the Cartan generator basis, we will sometimes choose to write the decomposition of twists in the flavor basis:  $(\Theta_\mu)_{ab} = \delta_{ab}\theta_\mu^a$ , where  $\theta_4^a = 0$  for all flavors. Furthermore, due to periodicity, we need only consider twist angles  $\theta_i^a$  in the range  $-\pi < \theta_i^a \leq \pi$ .

It is convenient to introduce quark fields  $\tilde{q}(x)$  defined by

$$\tilde{q}(x) = U^\dagger(x)q(x), \quad (3)$$

with

$$U(x) = e^{i\Theta_\mu x_\mu/L}. \quad (4)$$

The  $\tilde{q}(x)$  fields satisfy periodic boundary conditions. The quark part of the QCD Lagrangian can then be rewritten in the form

$$\mathcal{L} = \bar{\tilde{q}}(\tilde{\mathcal{D}} + M)\tilde{q}, \quad (5)$$

where the effect of twisting appears as a background gauge field

$$\tilde{D}_\mu = \partial_\mu + iB_\mu, \quad (6)$$

where  $B_\mu = \Theta_\mu/L$ .

To describe QCD at low energies, one turns to an effective field theory, chiral perturbation theory, that is written in terms of the pseudo-Goldstone bosons that appear from chiral symmetry breaking. As shown in [22], in the presence of twisting, this low-energy effective theory of QCD can be rewritten in terms of a modified coset field  $\tilde{\Sigma}(x)$  given by

$$\tilde{\Sigma}(x) = U^\dagger(x)\Sigma(x)U(x), \quad (7)$$

that satisfies periodic boundary conditions. The coset field  $\tilde{\Sigma}(x)$ , however, has nonvanishing charge in the background gauge field,  $B_\mu$ . In terms of the modified coset field, the chiral Lagrangian appears as

$$\mathcal{L} = \frac{f_\pi^2}{8} [\text{tr}(\tilde{D}_\mu \tilde{\Sigma} \tilde{D}_\mu \tilde{\Sigma}^\dagger) - \text{tr}(\tilde{\Sigma} \chi + \chi \tilde{\Sigma}^\dagger)], \quad (8)$$

where  $\chi$  is proportional to the quark mass and the covariant derivative is

$$\tilde{D}_\mu \tilde{\Sigma} = \partial_\mu \tilde{\Sigma} + i[B_\mu, \tilde{\Sigma}]. \quad (9)$$

From the Lagrangian in Eq. (8), we can deduce the propagator of the meson fields. For our general discussion, we begin by omitting the flavor structure of the propagator from our consideration. In a finite volume with dimensions  $L \times L \times L \times \beta$ , the meson propagator for the mode  $n_\mu = (\mathbf{n}, n_4)$  is proportional to

$$\frac{1}{(2\pi n_4/\beta)^2 + (2\pi\mathbf{n} + \Theta)^2/L^2 + m_\pi^2}, \quad (10)$$

where  $\mathbf{n} \in \mathbb{Z}^3$  and  $n_4 \in \mathbb{Z}$  due to the periodic boundary conditions and the  $\Theta$  term arises from the background gauge field. For power counting we will always assume  $\beta \sim 1/L \sim \epsilon$ . When one works in the  $\epsilon$  regime, where  $m_\pi L \ll 1$ , the zero-mode ( $n_\mu = 0$ ) of the finite-volume propagator ordinarily is strongly coupled. Twisting however has introduced an effective mass squared  $B_\mu^2 + m_\pi^2$  for the zero mode. Because the flavor-neutral mesons are unaffected by the twisting, there are always strongly coupled zero modes in the group manifold. In the twisted  $\epsilon$  regime all Goldstone boson zero modes are strongly coupled. Since the zero modes must be treated nonperturbatively, we separate the field into two pieces

$$\tilde{\Sigma}(x) = \tilde{\Sigma}_0 e^{2i\tilde{\phi}(x)/f_\pi}, \quad (11)$$

where  $\tilde{\Sigma}_0$  is the zero mode and the  $\tilde{\phi}$  contains the nonzero modes of the pion fields.

Returning to the Lagrangian in Eq. (8), we see that to lowest order the partition function in the twisted  $\epsilon$  regime is

$$Z = \int \mathcal{D}\tilde{\Sigma}_0 \exp\left\{\frac{\beta V f_\pi^2}{4} \text{tr}[B_\mu \tilde{\Sigma}_0 B_\mu \tilde{\Sigma}_0^\dagger + \Re(\chi \tilde{\Sigma}_0)]\right\}, \quad (12)$$

where  $V = L^3$ . We have dropped a  $B_\mu$  dependent constant which only modifies the normalization of the partition function and is physically irrelevant. Note that this partition function is very similar in form to that which arises when considering QCD with an isospin chemical potential [43–45]. However, an isospin chemical potential induces a  $B_\mu$  that is timelike rather than spacelike and the contribution to the action comes with the opposite sign. For our treatment of the zero modes in the  $SU(2)_L \times SU(2)_R$  and  $SU(3)_L \times SU(3)_R$  chiral theories, the expression for the partition function in Eq. (12) will be our starting point. We also will consider the partition function for the remnant  $\epsilon$  regime, where only the flavor-neutral mesons have strongly coupled zero modes. In this case, the matrix  $\tilde{\Sigma}_0$  belongs to the diagonal submanifold and only the quark mass term survives in Eq. (12).

### III. TWISTED $\epsilon$ REGIME OF $SU(2)$

In this section we consider the effects of twisted boundary conditions on the quark fields in two flavor  $\chi$ PT in the twisted  $\epsilon$  regime. The simplicity of the group manifold will allow us to reduce the zero-mode contribution to the partition function to a one-dimensional integral which is easily evaluated numerically. The dependence of the finite-volume quark condensate on twisting angle is then investigated. We also derive the partition function in the

remnant  $\epsilon$  regime when only the  $\pi^0$  zero mode is strongly coupled.

For two quark flavors, the general form of the background gauge field is

$$B_\mu = \text{diag}(B_\mu^u, B_\mu^d) = \frac{1}{2}(B_\mu^u + B_\mu^d) + \frac{1}{2}(B_\mu^u - B_\mu^d)\sigma_3. \quad (13)$$

The matrix integral appearing in Eq. (12) can largely be carried out due to the simple structure of the  $SU(2)$  group manifold. First notice the term proportional to the identity in Eq. (13) decouples from the zero-mode integration. To perform the remaining integration in the twisted  $\epsilon$  regime, we use a familiar parametrization of  $SU(2)$

$$\tilde{\Sigma}_0 = \cos\alpha + i\hat{n} \cdot \boldsymbol{\sigma} \sin\alpha, \quad (14)$$

where  $\hat{n}$  is a three-dimensional unit vector. With this choice for the arbitrary element of  $SU(2)$ , the group measure, normalized to unity, is

$$\int \mathcal{D}\tilde{\Sigma}_0 = \frac{1}{2\pi^2} \int d\Omega_{\hat{n}} \int_0^\pi d\alpha \sin^2\alpha, \quad (15)$$

and the partition function is straightforwardly evaluated.

The final result can be cast into the form of a one-dimensional integral over well-known functions. To this end, we define the dimensionless variables  $s$  and  $t$

$$s = \frac{1}{8} f_\pi^2 \beta V \text{tr}(\chi) = \frac{1}{4} f_\pi^2 \beta V m_\pi^2 = -\frac{m_u + m_d}{2} \langle \bar{q}q \rangle_\infty \beta V, \quad (16)$$

$$t = \frac{1}{4} (\mathbf{B}^u - \mathbf{B}^d)^2 f_\pi^2 \beta V = \frac{(\boldsymbol{\theta}^u - \boldsymbol{\theta}^d)^2}{4L^2} f_\pi^2 \beta V, \quad (17)$$

where  $m_\pi$  is the pion mass in the infinite volume limit. The variable  $s$  is the ordinary parameter relevant to the  $\epsilon$  regime [27], while the variable  $t$  contains the new effects due to twisting the quark fields at the boundary of the lattice. Notice  $t$  is zero only if in each spatial direction the quark phases at the boundary are pairwise identical. Furthermore in evaluating the matrix integral, we do not need to assume that the mass matrix is proportional to the identity. All results at this order in the chiral expansion depend only on  $\text{tr}(\chi)$ . Terms in  $\mathcal{L}^{(4)}$  lead to a departure from this result, but these are beyond the order we work.

The angular integral in the group measure can be done analytically. In terms of the variables  $t$  and  $s$ , the partition function to leading order in the twisted  $\epsilon$  regime is

$$Z(s, t) = \frac{1}{\sqrt{\pi}} \int_0^\pi d\alpha \frac{\sin\alpha}{\sqrt{t}} \text{Erfi}(\sqrt{t} \sin\alpha) \times \exp(2s \cos\alpha - t \sin^2\alpha), \quad (18)$$

where  $\text{Erfi}(x) = \text{Erf}(ix)/i$ , and  $\text{Erf}(x)$  is the standard error function. Untwisting the quark fields, i.e. for  $t = 0$ , we arrive at

$$Z(s, 0) = \frac{2}{\pi} \int_0^\pi d\alpha \exp(2s \cos\alpha) \sin^2\alpha, \quad (19)$$

which is the form of the ordinary  $SU(2)$  group integral in the  $\epsilon$  regime [27]. In terms of a modified Bessel function, we have  $Z(s, 0) = I_1(2s)/s$ .

In the twisted  $\epsilon$  regime,  $B_\mu \sim m_\pi \sim \epsilon^2$  and  $t/s \sim 1$ , but in the remnant  $\epsilon$  regime

$$\frac{t}{s} \propto \frac{B_\mu^2}{m_\pi^2} \sim \frac{1}{\epsilon^2}. \quad (20)$$

So the large  $t$  limit corresponds to the remnant  $\epsilon$  regime. Taking the asymptotic limit of the error function,

$$\lim_{x \rightarrow \infty} \frac{\text{Erfi}\sqrt{x}}{\sqrt{x}} = \frac{e^x}{\sqrt{\pi x}}, \quad (21)$$

we find the  $t$  dependence in Eq. (18) reduces to an overall multiplicative factor which can be pulled outside the integral. In general, one is interested in computing expectation values of operators which can be calculated by adding sources to the Lagrangian and then differentiating the logarithm of the partition function with respect to these sources. The condensate is obtained by differentiating  $\log Z(s, t)$  with respect to  $s$  [see Eq. (24) below]. So the multiplicative dependence on  $t$  is a trivial modification of the normalization of the path integral which can be ignored. Thus, for large  $t$ , the partition function is

$$Z(s) \propto \int_0^\pi d\alpha \exp(2s \cos\alpha) \propto I_0(2s). \quad (22)$$

The  $\pi^0$  zero mode has a mass  $\sim m_\pi \sim \epsilon^2$  but the charged pions have an effective mass  $\sim |B_\mu| \sim \epsilon$ . Physically, one expects to be able to integrate out the charged pion zero modes in this limit. The twisted  $\epsilon$  regime partition function should reduce to that of the remnant  $\epsilon$  regime, in which only the  $\pi^0$  zero mode is dynamical. The remnant  $\epsilon$  regime partition function is obtained using the parametrization

$$\tilde{\Sigma}_0 = \exp(i\alpha \sigma_3), \quad (23)$$

and the group integral measure is trivial since it is an integral over a  $U(1)$  subgroup of the coset  $SU(2)_L \times SU(2)_R / SU_V(2)$ . This immediately leads to a partition function identical to that in Eq. (22).

The quark condensates for the up and down quarks are identical,  $\langle \bar{u}u \rangle = \langle \bar{d}d \rangle$ , because the partition function depends only on the trace of the mass matrix  $\text{tr}(\chi)$ . We denote either of the condensates by  $\langle \bar{q}q \rangle$ . They are calculated by differentiating the partition function

$$\frac{\langle \bar{q}q \rangle}{\langle \bar{q}q \rangle_\infty} = \frac{1}{2} \frac{\partial}{\partial s} \log Z(s, t), \quad (24)$$

In Fig. 1, we show the dependence of the quark condensate on the twisting parameter  $t$ . For  $t = 0$ , the result is just that of the ordinary  $\epsilon$  regime of  $SU(2)$ . The condensate decreases with  $s$ , and vanishes as  $s \rightarrow 0$  due to the restoration

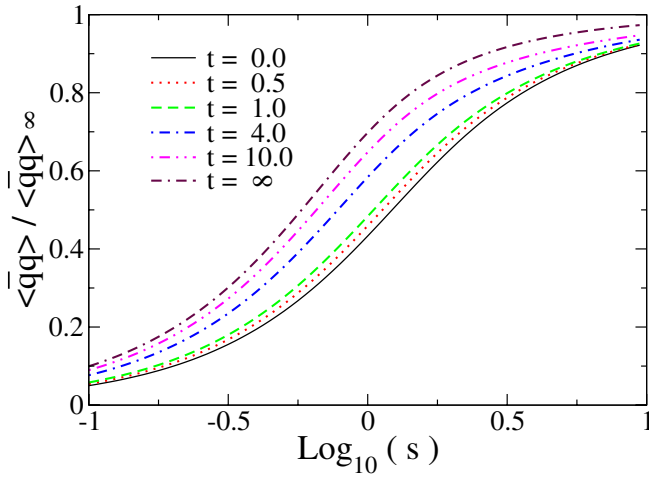


FIG. 1 (color online). The quark condensate of the  $SU(2)_L \times SU(2)_R$  theory with twisted boundary conditions is plotted as a function of  $s$ , for several values of the twisting parameter  $t$ . Results in the remnant  $\varepsilon$  regime correspond to the curve denoted  $t = \infty$ .

of chiral symmetry at finite volume. For  $t \neq 0$  there are twisted boundary conditions on the quark fields and the qualitative behavior of the condensate as a function of  $s$  is unchanged. The value of the finite-volume condensate, however, is altered and depends on the twisting variable  $t$ . As  $t$  becomes larger, the effective mass of the charged pion zero modes increases due to the twisting and these modes can no longer conspire to restore chiral symmetry. Therefore the condensate increases in magnitude with  $t$  for fixed  $s$ . When  $t/s$  is very large, the theory is in the remnant  $\varepsilon$  regime and only the  $\pi^0$  zero mode is relevant. The result for the remnant  $\varepsilon$  regime is denoted by the curve  $t = \infty$ .

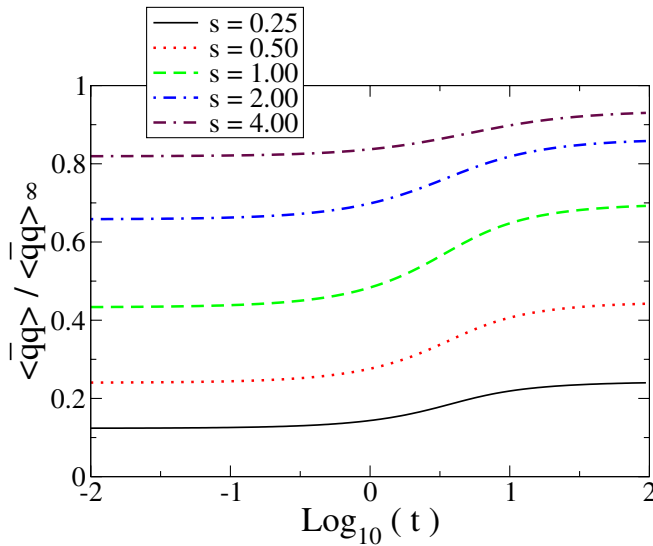


FIG. 2 (color online). The quark condensate of the  $SU(2)_L \times SU(2)_R$  theory with twisted boundary conditions is plotted as a function of the twisting parameter  $t$ , for several values of  $s$ .

We see that the behavior of the condensate for nonzero  $t$  approaches that of the remnant  $\varepsilon$  regime in the limit of large  $t$ . In Fig. 2 we plot the dependence of the quark condensate as a function of  $t$  for fixed  $s$ . Mapping out the dependence of the finite-volume condensate as a function of  $\theta^u - \theta^d$  for fixed four-volume and  $s$  gives one an alternate method to determine  $f_\pi$ . As  $s \rightarrow 0$  the condensate must vanish because of the restoration of chiral symmetry and therefore the value of the condensate is insensitive to the twisted boundary conditions. As  $s \rightarrow \infty$  one is approaching the infinite volume limit and all observables should be insensitive to boundary conditions. The condensate is most sensitive to twisted boundary conditions near  $s = 1$ .

#### IV. TWISTED $\varepsilon$ REGIME OF $SU(3)$

In this section, we investigate the consequences of twisted boundary conditions on QCD with three flavors of quark fields. The group integration over the  $SU(3)$  manifold is more complicated than  $SU(2)$ . Our formulas for the matrix integral in the most general case is an eight-dimensional integral which we do not know how to perform analytically. To simplify numerical analysis of the partition function, we work in the limit of massless up and down quarks and choose isospin symmetric boundary conditions. The partition function in this case can be reduced to a one-dimensional integral and the dependence of the strangeness condensate on twisting angles and strange quark mass can be easily calculated.

For the case of the  $SU(3)$  flavor group, the flavor-diagonal background gauge field is

$$B_\mu = \text{diag}(B_\mu^u, B_\mu^d, B_\mu^s) = B_\mu^0 + B_\mu^3 \lambda_3 + B_\mu^8 \lambda_8, \quad (25)$$

where  $B_\mu^0 = \frac{1}{3}(B_\mu^u + B_\mu^d + B_\mu^s)$ ,  $B_\mu^3 = \frac{1}{2}(B_\mu^u - B_\mu^d)$ , and  $B_\mu^8 = \frac{1}{2\sqrt{3}}(B_\mu^u + B_\mu^d - 2B_\mu^s)$ . In Eq. (12), any terms involving  $B_\mu^0$  decouple from the group integral. For the arbitrary group element of  $SU(3)$ , we use a convenient form [46,47] that is a generalization of the Euler angle decomposition,

$$\tilde{\Sigma}_0 = e^{-i\lambda_3\alpha} e^{i\lambda_2\beta} e^{-i\lambda_3\gamma} e^{i\lambda_5\psi} e^{-i\lambda_3a} e^{i\lambda_2b} e^{-i\lambda_3c} e^{-i\lambda_8\phi}. \quad (26)$$

With this decomposition, the invariant volume element of the  $SU(3)$  group is [46–48]

$$\int \mathcal{D}\tilde{\Sigma}_0 \propto \int_0^{\sqrt{3}\pi} d\phi \int_0^\pi d\alpha d\gamma d\psi d\beta d\psi \sin 2\beta \sin 2b \sin 2\psi \sin^2 \psi. \quad (27)$$

(Note that in this case we have not chosen to normalize the group integral to 1.)

For the moment, let us consider three independent flavor twists and three nondegenerate quark masses. In this general case, we can write the partition function in the twisted  $\varepsilon$  regime as a function of the quark mass dependent variables  $s^a = \frac{1}{4}\chi^a f_\pi^2 \beta V$  and the various combinations of flavor twists,  $t^{ab} = \frac{1}{4}\mathbf{B}^a \cdot \mathbf{B}^b f_\pi^2 \beta V$ . We find the partition

function has the form

$$Z(s^a, t^{ab}) = N \int \mathcal{D}\tilde{\Sigma}_0 \exp[f(s^u, s^d, s^s) + g(t^{33}, t^{38}, t^{88})], \quad (28)$$

where the quark mass dependent term in Eq. (12) contributes to the function  $f(s^u, s^d, s^s)$ , which is given by

$$f(s^u, s^d, s^s) = s^s \cos\psi \cos\frac{2\phi}{\sqrt{3}} + \left[ s^d \cos\left(a + c + \alpha + \gamma - \frac{\phi}{\sqrt{3}}\right) + s^u \cos\psi \cos\left(a + c + \alpha + \gamma + \frac{\phi}{\sqrt{3}}\right) \right] \cos b \cos\beta - \left[ s^u \cos\left(a - c - \alpha + \gamma - \frac{\phi}{\sqrt{3}}\right) + s^d \cos\psi \cos\left(a - c - \alpha + \gamma + \frac{\phi}{\sqrt{3}}\right) \right] \sin b \sin\beta, \quad (29)$$

and the term in Eq. (12) which depends on the background gauge field contributes to the function  $g(t^{33}, t^{38}, t^{88})$ , which is given by

$$g(t^{33}, t^{38}, t^{88}) = \frac{1}{2} t^{33} [(3 + \cos 2\psi) \cos 2\beta \cos 2b - 4 \cos(2a + 2\gamma) \cos\psi \sin 2\beta \sin 2b] - \sqrt{3} t^{38} (\cos 2\beta + \cos 2b) \sin^2 \psi + \frac{3}{2} t^{88} \cos 2\psi. \quad (30)$$

The full expression for the partition function in Eq. (28) is an eight-dimensional integral which appears difficult to evaluate analytically in the most general case. We will make two assumptions which greatly simplify the evaluation of the partition function. It is convenient to choose isospin symmetric boundary conditions with  $B_\mu^d = B_\mu^u$ . In this case, we have

$$g(t') = \frac{t'}{2} \cos 2\psi, \quad (31)$$

where  $t' = \frac{1}{4}(\mathbf{B}^u - \mathbf{B}^s)^2 f_\pi^2 \beta V$ . Secondly, we make the physically relevant approximation of neglecting up and down quarks masses while letting the strange quark mass be nonzero. Then the action only depends on the angles  $\phi$  and  $\psi$  and all but one integral can be done analytically:

$$Z(s^s, t') = N' \int_0^{\sqrt{3}\pi} d\phi \int_0^{\pi/2} d\psi \sin 2\psi \sin^2 \psi \exp\left(s^s \cos\psi \cos\frac{2\phi}{\sqrt{3}} + \frac{t'}{2} \cos 2\psi\right) = N'' \int_0^1 dx x(1-x^2) I_0(s^s x) e^{t'(x^2-1/2)}, \quad (32)$$

where  $I_0(x)$  is a modified Bessel function.

The strangeness condensate,  $\langle \bar{s}s \rangle$ , is given by

$$\frac{\langle \bar{s}s \rangle}{\langle \bar{s}s \rangle_\infty} = \frac{\partial}{\partial s^s} \log Z(s^s, t'), \quad (33)$$

where the corresponding condensate in the infinite volume limit is denoted by  $\langle \bar{s}s \rangle_\infty$ . In Fig. 3, we show the dependence of the strangeness condensate on the twisting parameter  $t'$ . The result for  $t' = 0$ , corresponding to the case of periodic boundary conditions, is the finite-volume behavior of the condensate in the ordinary  $\varepsilon$  regime. Like the  $\langle \bar{q}q \rangle$  condensate in the  $SU(2)_L \times SU(2)_R$  theory, the  $\langle \bar{s}s \rangle$  condensate decreases monotonically with  $m_s$ . When  $t'$  is nonzero, the theory is in the twisted  $\varepsilon$  regime and the qualitative behavior as a function of  $s^s$  is unchanged. However, the flavor nondiagonal zero modes become less important than the flavor-diagonal modes. The condensate is larger in the presence of twisted boundary conditions.

The greatest enhancement is achieved when  $t'/s^s \gg 1$ , which is the remnant  $\varepsilon$  regime.

Although we have not been able to analytically derive the large  $t'$  limit of the strangeness condensate directly from Eqs. (32) and (33), we can treat the remnant  $\varepsilon$  regime exactly when  $m_u = m_d = 0$ . In the remnant  $\varepsilon$  regime, only the  $\pi^0$  and  $\eta$  zero modes remain strongly coupled. The integral over the  $SU(3)_L \times SU(3)_R/SU(3)_V$  coset reduces to integrals over the  $U(1)$  diagonal subgroups. Therefore, the measure is trivial and  $\tilde{\Sigma}_0$  can be parametrized by the diagonal matrix  $\tilde{\Sigma}_0 = \text{diag}(e^{i\theta_1}, e^{i\theta_2}, e^{-i(\theta_1+\theta_2)})$ . Thus, the partition function in the remnant  $\varepsilon$  regime is

$$Z(s^a) = N \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \times \exp[s^u \cos\theta_1 + s^d \cos\theta_2 + s^s \cos(\theta_1 + \theta_2)]. \quad (34)$$

To compare with our numerical results in the twisted  $\varepsilon$

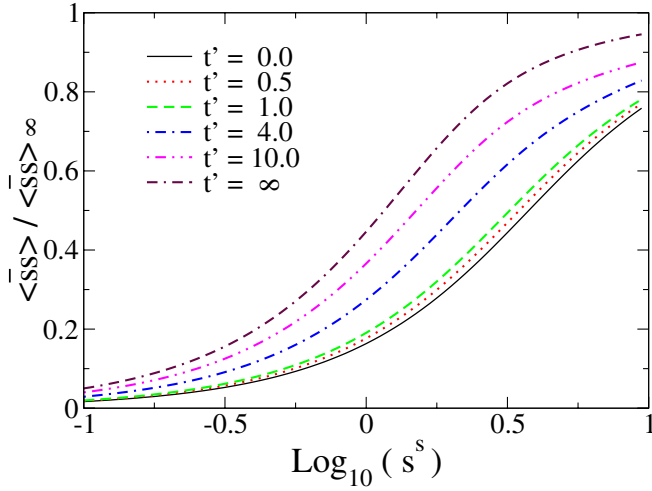


FIG. 3 (color online). The strangeness condensate in the  $SU(3)_L \times SU(3)_R$  theory with twisted boundary conditions as a function of  $s^s$ , for several values of the twisting parameter  $t'$ . The remnant  $\varepsilon$  regime corresponds to the curve denoted  $t' = \infty$ . Note that  $B_u = B_d$  and  $m_u = m_d = 0$ .

regime, we set  $s^u = s^d = 0$ , and find  $Z(s^s) \propto I_0(s^s)$ . The resulting strangeness condensate is labeled by  $t' = \infty$  in Fig. 3.

## V. TWISTED QUARKS IN FIXED TOPOLOGY

In this section, we discuss the effect of twisted boundary conditions on the partition function in sectors of fixed topological charge. If  $Z_\nu$  corresponds to the partition function in a sector with topological charge  $\nu$  then  $Z_\nu/Z$  can be interpreted as the probability of finding the gauge configuration with topological charge  $\nu$ . This can be computed by introducing a  $\theta$  term in the chiral Lagrangian and computing the Fourier transform of the partition function with respect to  $\theta$ . Reference [42] showed that the QCD partition function is dominated by vanishing or small  $\nu$  in the  $\varepsilon$  regime. We study whether this conclusion is modified in the presence of twisted boundary conditions. For simplicity we consider only the  $SU(2)_L \times SU(2)_R$  theory with  $m_u = m_d$ .

In the twisted  $\varepsilon$  regime, the partition function for vacuum angle  $\theta$  is given by

$$Z(\theta) = \int \mathcal{D}\tilde{\Sigma}_0 \exp \left\{ \frac{\beta V f_\pi^2}{4} \text{tr} [B_\mu \tilde{\Sigma}_0 B_\mu \tilde{\Sigma}_0^\dagger + \Re(e^{i\theta/2} \chi \tilde{\Sigma}_0)] \right\}, \quad (35)$$

where we have specialized to the case of two flavors. In a sector with fixed topological charge  $\nu$ , the corresponding partition function is

$$Z_\nu = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-i\nu\theta} Z(\theta), \quad (36)$$

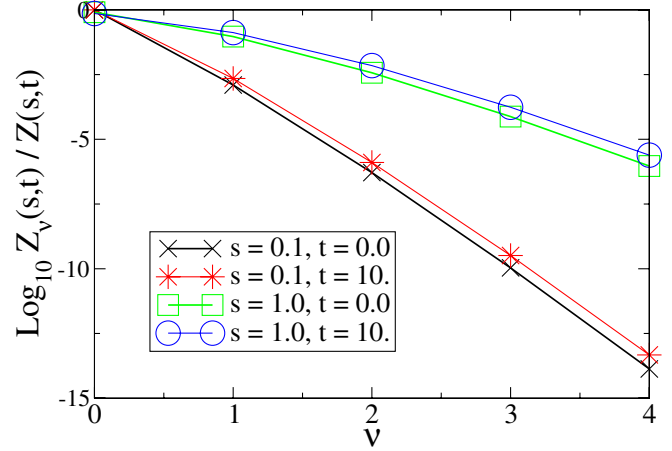


FIG. 4 (color online). The partition function for fixed topological charge. We plot  $\text{log}_{10}[Z_\nu(s,t)/Z(s,t)]$  as a function of  $\nu$  for different  $s$  and  $t$ . The solid lines are provided merely to guide the eye.

and can be straightforwardly evaluated.<sup>3</sup> We find

$$Z_\nu(s,t) = \frac{1}{\sqrt{\pi}} \int_0^\pi d\alpha \frac{\sin\alpha}{\sqrt{t}} \text{Erfi}(\sqrt{t} \sin\alpha) \times e^{-t \sin^2 \alpha} I_{2\nu}(2s \cos\alpha). \quad (37)$$

Note that  $Z_\nu(s,t) = Z_{-\nu}(s,t)$ . It is easy to show that in the limit  $t \rightarrow 0$ , we recover the result [42]

$$Z_\nu(s,0) = I_\nu(s)^2 - I_{\nu+1}(s)I_{\nu-1}(s).$$

In Fig. 4 the logarithm of the ratio  $Z_\nu(s,t)/Z(s,t)$  is plotted for  $\nu = 0$  through  $\nu = 4$ . In this plot we show the result for two different values of  $s$  with and without twisted boundary conditions. We see that the dominance of the sector with zero topological charge in the  $\varepsilon$ -regime is not modified by twisting. The numerical value of  $Z_\nu(s,t)/Z(s,t)$  changes little between  $t = 0$  and  $t = 10$ .

## VI. SUMMARY

In this paper, we have investigated the effects of twisted boundary conditions on the quark condensate in small volumes. We worked in the twisted  $\varepsilon$  regime of chiral perturbation theory where  $1/L \sim \varepsilon$ ,  $B_\mu \sim m_\pi \sim \varepsilon^2$  and all Goldstone boson zero modes are strongly coupled. The partition function and quark condensate were computed to leading order by performing the path integral over these zero modes. We also investigated the remnant  $\varepsilon$  regime, where  $1/L \sim B_\mu \sim \varepsilon$ ,  $m_\pi \sim \varepsilon^2$ . In this case only the flavor-neutral mesons are strongly coupled and the

<sup>3</sup>A similar partition function arises in the case of an isospin chemical potential [44]. In particular, setting  $n = 1$ , taking the variable  $z$  to be real, and replacing  $\mu^2 \rightarrow -\mu^2$  in Eq. (102) of [44], gives a partition function that is essentially identical to our  $Z_0(s,t)$ . For  $n = 1$  the partition function is expressed in terms of a one-dimensional integral in Eq. (109) of [44].

contribution from these modes dominates the partition function. It is the flavor-neutral zero modes that lead to a restoration of chiral symmetry at small volumes in the remnant  $\varepsilon$  regime.

The value of the quark condensate in small volumes affects the masses of particles. For example, the pion mass is given by

$$m_\pi^2 = \frac{\text{tr}(\chi) \langle \bar{q}q \rangle}{2 \langle \bar{q}q \rangle_\infty}, \quad (42)$$

and the masses of heavy particles, such as the nucleon [49], pick up an additive renormalization,

$$m_N = m_0 - \alpha \text{tr}(\chi) \frac{\langle \bar{q}q \rangle}{\langle \bar{q}q \rangle_\infty}. \quad (43)$$

When one imposes twisted boundary conditions on the quark fields, particle masses are modified since  $\langle \bar{q}q \rangle$  is larger relative to its value in the absence of twisting. Of course, the pion mass vanishes at very small volumes in any case.

Lattice calculation of the dependence of quark condensates and particle masses on twisted boundary conditions can be used to test the predictions of twisted chiral perturbation theory. Moreover because the kinetic energy term contributes to the twisted partition function, it is in princi-

ple possible to determine both the infinite volume condensate and the pion decay constant from numerically determining the finite-volume condensate as a function of the twist angles and volume. Lastly, we showed that sectors with zero topological charge remain the dominant contributors to the partition function in the twisted and remnant  $\varepsilon$  regimes.

For the results in this paper to be useful in actual simulations, it may be necessary to extend our calculations to include effects due to quenching or partial quenching as well as perturbative loop corrections from nonzero modes. Note that the simplicity of the zero-mode manifold in the remnant  $\varepsilon$  regime may make it easier to compute the partition function for quenched and partially quenched theories with twisted quarks. It would also be interesting to examine other correlation functions, especially two point functions of currents. We hope this paper will stimulate further numerical and analytical work in this novel regime of QCD.

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