

## Anomalous Chiral Symmetry Breaking above the QCD Phase Transition

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We study the anomalous breaking of  $U_A(1)$  symmetry just above the QCD phase transition for zero and two flavors of quarks, using a staggered fermion, lattice discretization. The properties of the QCD phase transition are expected to depend on the degree of  $U_A(1)$  symmetry breaking in the transition region. For the physical case of two flavors, we carry out extensive simulations on a  $16^3 \times 4$  lattice, measuring a difference in susceptibilities which is sensitive to  $U_A(1)$  symmetry and which avoids many of the staggered fermion discretization difficulties. The results suggest that anomalous effects are at or below the 15% level. [S0031-9007(99)08688-3]

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The breaking of classical  $U_A(1)$  chiral symmetry by quantum effects is a theoretical phenomenon of considerable physical importance which has direct implications on the order of the finite temperature, QCD phase transition. If we consider only the two light  $u$  and  $d$  quarks, anomalous symmetry breaking reduces the flavor symmetry from  $U(2) \times U(2)$  to  $SU(2) \times SU(2) \times U_B(1) \times Z_A(2)$ . It is only this reduced symmetry that is consistent with second-order, critical behavior [1]. Although present lattice simulations suggest that the QCD phase transition is indeed second order for two flavors, it is an important consistency check to establish the required anomalous  $U_A(1)$  symmetry breaking directly. In addition, the size of these symmetry breaking effects will determine the width in temperature and quark mass of the region showing universal critical behavior.

The plasma phase of QCD is a particularly good place to study the axial anomaly. For  $T < T_c$ , the dynamical breaking of chiral symmetry obscures the effects of the axial anomaly. For  $T > T_c$ , chiral symmetry is restored and thermal Greens' functions are explicitly symmetric under  $SU(N_f) \times SU(N_f)$  transformations. We can then look directly for anomalous symmetry breaking by comparing Greens functions that are related by the anomalous  $U_A(1)$  symmetry.

Such breaking of global  $U_A(1)$  symmetry, associated with a zero-momentum Ward identity, is especially interesting, since at zero momentum the anomalous term in the chiral Ward identity becomes  $N_f$  times the topological charge  $\nu$ , a quantity which vanishes to all orders in conventional perturbation theory. The  $\eta'$  mass in QCD and the nonconservation of the baryon number in the standard model are other examples in which such nonperturbative anomalous effects should occur [2].

This sort of anomalous symmetry breaking can be understood from two perspectives: (i) As the physical remnant of an ultraviolet ambiguity in the theory. Here modifications made to regulate the divergences present in the continuum gauge theory necessarily introduce explicit chiral symmetry breaking whose effects remain visible, even on energy scales small compared to those of

the regulator. (ii) As resulting from an infrared singularity which permits chiral asymmetry to survive the chiral limit of vanishing fermion mass. While chiral symmetry breaking effects might naively be expected to be proportional to the explicit quark mass,  $m$ , the presence of infrared singular,  $1/m$  behavior can allow such chirally asymmetric effects to remain even in the  $m \rightarrow 0$  limit. In a semiclassical calculation, such  $1/m$  behavior appears for gauge backgrounds with fermion zero modes. These two views are related by the Atiyah-Singer index theorem [3].

Most lattice calculations [4] explore the first approach, studying explicit chiral symmetry breaking inherent in the lattice regulation which should reduce to anomalous effects as the continuum limit is taken [5]. In this paper we explore the second approach, searching for anomalous asymmetries that arise from infrared singularities in the limit of small quark mass. For lattice calculations these two approaches are not equivalent since the Atiyah-Singer theorem applies only in the limit of an infinite number of degrees of freedom.

It is important to pursue both methods. The first approach may overestimate anomalous effects, confusing them with simple lattice artifacts which vanish in the continuum limit. The second approach may miss anomalous effects since infrared singularities are often softened by lattice effects, e.g., the zero-mode shift of Smit and Vink [6], and become apparent only as  $a \rightarrow 0$ .

The question of anomalous symmetry breaking above  $T_c$  has now been studied by a number of groups. For a general review, see the article of Laermann [7]. Preliminary versions of our results can be found in Ref. [8], while an alternative calculation, also taking approach (ii), can be found in Bernard *et al.* [9]. Finally, Kogut *et al.* [10] use a combination of methods examining signals for anomalous symmetry breaking of both types (i) and (ii) above.

In this paper, we study both zero- and two-flavor QCD, just above  $T_c$ . For  $N_f = 0$ , anomalous effects are expected in the chiral condensate,  $\langle \bar{q}q \rangle$ , while for  $N_f = 2$  we must examine a more infrared singular,  $U_A(1)$ -noninvariant quantity, here a difference of isovector

susceptibilities which we refer to as  $\omega = \chi_P - \chi_S$  where

$$\chi_P = \frac{1}{2\Omega} \int d^4x d^4y \langle \bar{\chi} \tau^j i \gamma^5 \chi(x) \bar{\chi} \tau^j i \gamma^5 \chi(y) \rangle \quad (1)$$

for space-time volume  $\Omega$  and flavor generator  $\tau^j$ . The scalar susceptibility  $\chi_S$  is defined similarly, by omitting the internal  $i\gamma^5$  factors.

We adopt the staggered fermion, lattice discretization. This is the approach used most successfully to date in finite temperature, lattice QCD studies. While the quantity  $\langle \bar{q}q \rangle$  can be calculated directly using this formalism, the more physically interesting  $\omega = \chi_P - \chi_S$  cannot. Direct definitions of  $\chi_P$  and  $\chi_S$  using staggered fermions will necessarily introduce ambiguities, with potentially large lattice artifacts obscuring the anomalous effects of interest.

Here, we take an indirect approach, expressing  $\omega$ , in the continuum, as a spectral integral whose singular behavior as  $m \rightarrow 0$  gives rise to anomalous symmetry breaking. We then demonstrate that this spectral integral can be directly evaluated using staggered lattice fermions and use this result to provide a lattice calculation of  $\omega$ .

Consider the spectral representations,

$$\langle \bar{q}q \rangle = -2m_\zeta \int_0^\infty d\lambda \frac{\rho(\lambda, g^2, m)}{\lambda^2 + m_\zeta^2} \Big|_{m_\zeta=m}, \quad (2a)$$

$$\omega = 4m^2 \int_0^\infty d\lambda \frac{\rho(\lambda, g^2, m)}{(\lambda^2 + m^2)^2}. \quad (2b)$$

Here  $\rho(\lambda, g^2, m)$  is the average density of Dirac eigenvalues  $\lambda$ . The first formula is due to Banks and Casher [11] and the second is derived in a similar fashion. In Eq. (2a) we distinguish the fermion mass that appears in the fermion line attached to  $q$  and  $\bar{q}$ ,  $m_\zeta$ , from that entering through the fermion determinant,  $m$ . The factors of  $m$  or  $m_\zeta$  in the numerators of Eq. (2) reflect the chiral symmetry breaking character of  $\langle \bar{q}q \rangle$  and  $\omega$ . However, an anomalous, small-mass limit can result if the integral over  $\lambda$  is sufficiently singular for small  $\lambda$ .

Now let us investigate what might be expected for these quantities in continuum QCD. For  $T > T_c$ , the small mass limit of  $\langle \bar{q}q \rangle$  and  $\omega$  in the continuum theory can be analyzed for both the case of very small volume and in the limit of infinite volume. For finite volume, the Dirac spectrum will be discrete for each gauge configuration in the path integral. The only nonzero contributions to either  $\langle \bar{q}q \rangle$  or  $\omega$  as  $m \rightarrow 0$  will come from gauge configurations with at least one exact Dirac zero mode. In very small volumes, these zero modes can be predicted semiclassically and give the anomalous, small-mass behaviors:  $\langle \bar{q}q \rangle \sim 1/m$ , for  $N_f = 0$  and  $\omega \sim \text{const}$ , for  $N_f = 2$ .

The case where  $V \rightarrow \infty$  first is more interesting and can be analyzed using the methods of Leutwyler and Smilga [12]. Above  $T_c$ , there are no massless modes so the free energy should be proportional to the volume and analytic in the fermion mass,

$$Z \approx \exp \Omega [F_0 + F_2 \text{tr} M^\dagger M + G \text{Re}(e^{i\theta} \det M)], \quad (3)$$

where  $M$  is the complex fermion mass matrix and  $\theta$  the usual theta parameter. Defining the topological susceptibility as  $\chi_{\text{top}} = -\partial^2/\partial\theta^2 \ln Z$ , one easily derives  $\chi_{\text{top}} = \Omega G m^{N_f}$  for  $\theta = 0$  and  $M = mI$ , a multiple of the identity.

We can similarly obtain expressions for  $\langle \bar{q}q \rangle$  and  $\omega$ ,

$$\langle \bar{q}q \rangle = -\frac{1}{N_f \Omega} \frac{\partial}{\partial m} \ln Z(M) = -2F_2 m - G m^{N_f-1}, \quad (4a)$$

$$\omega = \frac{1}{\Omega} \left[ \frac{\partial^2}{\partial m_r^2} - \frac{\partial^2}{\partial m_i^2} \right] \ln Z(M) = 2G m^{N_f-2}, \quad (4b)$$

where in Eq. (4a) we have divided by  $N_f$  to define  $\langle \bar{q}q \rangle$  as coming from a single fermion species while in Eq. (4b) we have used a complex  $M = mI + (m_r^j + im_i^j)\tau^j$ .

If we make the possibly reasonable assumption that the quenched value of  $\langle \bar{q}q \rangle$  can be obtained as the  $N_f \rightarrow 0$  limit of Eq. (4a), then we can combine Eq. (4) with the formula for  $\chi_{\text{top}}$  to obtain

$$\begin{aligned} N_f = 0: \quad \langle \bar{q}q \rangle &= -\frac{1}{m} \frac{\chi_{\text{top}}}{\Omega} \sim \frac{1}{m}, \\ N_f = 2: \quad \omega &= \frac{2}{m^2} \frac{\chi_{\text{top}}}{\Omega} \sim \text{const}. \end{aligned} \quad (5)$$

The last relation is of particular interest, implying that above  $T_c$  the quantity  $\omega$  provides an alternative measure of the topological susceptibility. As is shown below,  $\omega$  can be easily determined using lattice methods, without the normal difficulties of defining topological winding on a discrete lattice.

We will now compare these continuum expectations with lattice calculations. Because of the remnant chiral symmetry of staggered fermions, Eq. (2a) is also valid on the lattice, allowing us to relate  $\langle \bar{\chi}\chi \rangle$  and  $\rho$ , where  $\chi$  is the single component, staggered fermion field. Viewing  $\langle \bar{q}q \rangle$  as a function of  $m$  and  $m_\zeta$ , we can express  $\omega$  as a function of  $\langle \bar{q}q \rangle$  and then use this continuum result to define  $\omega$  on the lattice,

$$\omega = -\frac{1}{m} \langle \bar{\chi}\chi \rangle + \frac{\partial}{\partial m_\zeta} \langle \bar{\chi}\chi \rangle \Big|_{m_\zeta=m}, \quad (6)$$

where these two terms correspond precisely to the terms in the difference  $\omega = \chi_P - \chi_S$ . In the remainder of this paper we quote values of  $\omega$ ,  $\chi_P$ , and  $\chi_S$  normalized according to Eq. (6) where  $\langle \bar{\chi}\chi \rangle$  is normalized to behave as  $-1/m$  in the large mass limit.

First consider  $N_f = 0$ . In Fig. 1 we show  $\langle \bar{\chi}\chi \rangle$  for two distinct phases distinguished by the complex phase of the Wilson line,  $\langle W \rangle$ , computed at  $\beta = 5.71$ , just above  $\beta_c = 5.6925$ . (Recall that the Wilson line,  $W$ , is the volume average of the trace of the ordered product of link variables along a line in the time direction.) For the case where  $\langle W \rangle$  is real, we see the power law  $\sim m^{0.76}$  for both  $16^3$  and  $32^3$  volumes suggesting this power-law

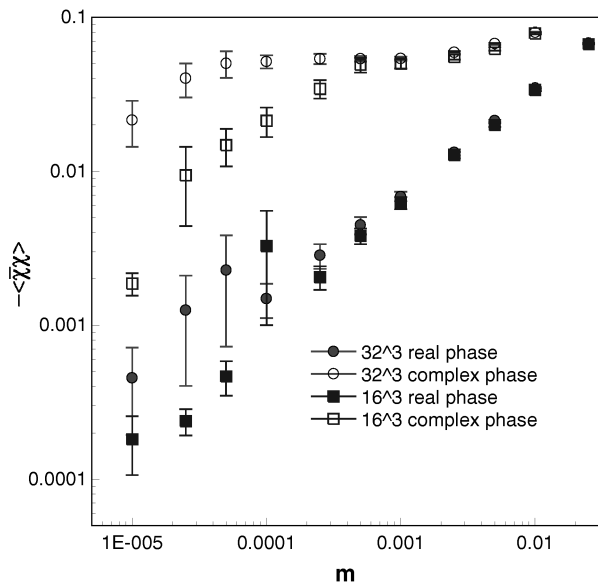


FIG. 1. The chiral condensate  $\langle \bar{\chi}\chi \rangle$  plotted as a function of quark mass for a pure gauge calculation on  $16^3 \times 4$  and  $32^3 \times 4$  lattices. The real phase (closed points) is the most physical [ $\det(D - m)$  is largest for this phase]. No evidence is seen for the expected anomalous behavior,  $\langle \bar{\chi}\chi \rangle \sim m^{-1}$  as  $m \rightarrow 0$ .

description holds in the infinite volume limit. We see no sign of the anomalous  $1/m$  behavior in  $\langle \bar{\chi}\chi \rangle$  expected in the continuum.

For the case of complex  $\langle W \rangle$ , we see an unexpected spontaneous breaking of chiral symmetry above  $T_c$ , with  $\langle \bar{\chi}\chi \rangle$  approaching a constant as  $m$  decreases. The eventual decrease in  $\langle \bar{\chi}\chi \rangle$  for very small  $m \leq m_{\min}$  is the normal finite-volume behavior expected with spontaneous symmetry breaking, with  $m_{\min} \langle \bar{\chi}\chi \rangle V/T \approx 1$  for both volumes.

Next we examine  $\omega$  and the more physical case of two flavors, at  $\beta = 5.3$ , just above  $\beta_c$  (recall  $\beta_c \approx 5.265$  for  $N_t = 4$  and  $ma = 0.01$ ), on a  $16^3 \times 4$  lattice for five different values of the dynamical quark mass. The results are summarized in Table I and plotted in Fig. 2. [Both  $\omega$  and  $\chi_S$  are computed from analytic derivatives of cubic spline fits to the  $m_\zeta$  dependence of  $\bar{\chi}\chi(m_\zeta)/m_\zeta$  and  $\bar{\chi}\chi(m_\zeta)$ , respectively.] This figure shows the chiral condensate,  $\langle \bar{\chi}\chi \rangle$  approaching zero linearly as is expected for  $\beta > \beta_c$ . Likewise,  $\chi_P$  shows the expected regular, constant behavior as  $m \rightarrow 0$ . However, rather than showing the anomalous behavior,  $\omega \sim \omega_0 + \omega_2 m^2$ , expected from Eq. (5), Fig. 2 suggests a nearly linear  $\omega$  as  $m$  goes to zero.

Four fitted curves are also shown in Fig. 2. The two linear fits to  $\langle \bar{\chi}\chi \rangle$  and  $\omega$  have a  $\chi^2/\text{d.o.f}$  of 2.2 and 2.7, respectively. Both of these fits are constrained to vanish at  $m = 0$ . If that constraint is dropped for the  $\omega$  fit, the intercept moves upward slightly to 0.15(5) and the  $\chi^2/\text{d.o.f}$  falls to 0.34. A fit to the expected form  $\omega_0 + \omega_2 m^2$  is worse, with a  $\chi^2/\text{d.o.f}$  of 3.4 and an intercept,  $\omega_0 = 0.54(3)$ .

TABLE I. Our  $\beta = 5.3$ ,  $16^3 \times 4$  results for two flavors of dynamical quark with mass  $m$ . Run length is the number of time units in the hybrid, “R”-algorithm evolution after 200 time units were discarded. These quantities are normalized in a manner consistent with Eq. (6) with  $\bar{\chi}\chi$  defined so that it behaves as  $1/ma$  for large  $ma$ . The time step sizes used with the R algorithm are  $\Delta\tau = 0.03125$  for  $ma = 0.005$ ;  $\Delta\tau = 0.007125$  for  $ma = 0.01$ ; and  $\Delta\tau = 0.01$  for the three larger masses.

$ma$	Run length	$\langle \bar{\chi}\chi \rangle$	$\chi_S$	$\omega$
0.005	4464	0.02256(21)	3.945(43)	0.559(37)
0.01	2550	0.04374(50)	3.369(68)	0.932(56)
0.015	2600	0.06517(82)	3.010(52)	1.322(62)
0.02	2992	0.0896(10)	2.697(34)	1.722(62)
0.025	3072	0.1141(38)	2.38(11)	2.24(12)

While these results are consistent with those reported by Bernard *et al.* [9], our conclusions are different. That calculation examines a smaller lattice spacing than considered here but with larger statistical errors. Their analysis adopts the quadratic small-mass dependence for  $\omega$ . While, as implied by Eqs. (3) and (4b), this quadratic behavior is expected on physical grounds for  $N_f = 2$ , it is only guaranteed mathematically in the unphysical limit where  $m$  vanishes at fixed lattice spacing. For example, nonuniformity in the limit of vanishing  $a$  and  $m$  is actually expected in the case of three flavors: for  $N_f = 3$  Eq. (4b) implies a linear behavior for  $\omega(m)$  in conflict with the quadratic dependence expected from the functional form of the path integral at finite  $a$ . Thus, the validity of the expected quadratic behavior needs to be established numerically for the mass range of interest. Unfortunately, our poor quadratic fit does not provide this needed justification.

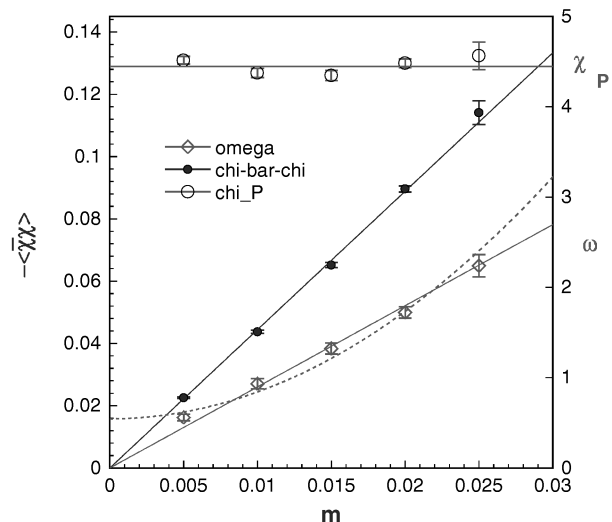


FIG. 2. The quantity  $\omega$ , which directly measures anomalous symmetry breaking, plotted versus fermion mass,  $ma$ . Also shown are the chiral condensate  $\langle \bar{\chi}\chi \rangle$  and the pseudoscalar susceptibility  $\chi_P$ . We studied a  $16^3 \times 4$  lattice at  $\beta = 5.3$ , just above  $\beta_c$ .

From Fig. 2 one observes that for quark masses in the range  $0.01 \leq m \leq 0.025$ , our results are consistent with an unusual but nonanomalous, linear behavior  $\omega \sim m$ . At our smallest mass, 0.005,  $\omega$  is significantly higher than such a linear extrapolation, suggesting that anomalous effects may be emerging. However, such effects are clearly quite small and occur for quark masses that are below those used in present studies of QCD thermodynamics, suggesting little connection between this anomalous behavior and the observed second-order QCD phase transition.

In order to describe the physical size of a possible nonzero value of  $\omega|_{m=0}$ , we must address the potential cutoff dependence of the quantities being discussed. While a thorough analysis of this question lies beyond the scope of the present paper [13], there are two issues that are important to recognize. First, the  $m = 0$  intercept of  $\omega$  requires the same  $\ln(a)$ -dependent, multiplicative renormalization as the inverse square of the quark mass  $m$ , as is suggested by Eq. (5). We will ignore such a factor for our present rough estimate, since this factor should be of the order of 1 for current lattice spacings.

Since  $\omega$  is the difference of  $\chi_P$  and  $\chi_S$ , it is natural to compare  $\omega$  to either of these quantities. However, both quantities contain a  $1/a^2$  piece when evaluated in physical units. Thus, we choose to compare  $\omega$  to a quantity we will call  $\tilde{\omega}$ , obtained as the difference between  $\chi_P$  evaluated at  $\beta = 5.3$  and  $\chi_S$  evaluated at  $\beta = 5.245$ , just below the transition,

$$\tilde{\omega} = \left. \frac{\langle \bar{\chi}\chi \rangle}{m} \right|_{\beta=5.3} - \left. \frac{\partial \langle \bar{\chi}\chi \rangle}{\partial m_\zeta} \right|_{\beta=5.245}. \quad (7)$$

Such a subtraction removes the unwanted, quadratically divergent  $1/a^2$  term at tree level and leaves an expression finite up to an  $O(1)$ ,  $\ln(a)$ -dependent multiplicative factor and a much smaller  $1/a^2$  term suppressed by the factor  $(5.3 - 5.245)$ . Note, both  $\omega$  and  $\tilde{\omega}$  would share the same  $1/m$  divergence as  $T \rightarrow T_c^+$  if the anomalous breaking takes the expected form:  $\chi_P \sim 1/m$ ,  $\chi_S \sim \text{const}$  as  $T$  approaches  $T_c$  from above. Thus, in the case of anomalous symmetry breaking and  $T \rightarrow T_c^+$  we expect  $\omega/\tilde{\omega} = 1$ . We find  $\omega/\tilde{\omega} \sim 15\%$  where for  $\omega$  we use the intercept 0.54 above and  $\partial \langle \bar{\chi}\chi \rangle / \partial m_\zeta|_{\beta=5.245} = 0.97$  [13].

Within the expected critical region, the light modes  $(\vec{\pi}, \sigma)$  should be much less massive than the nonuniversal degrees of freedom suggesting  $\omega/\tilde{\omega} \sim 1$ , not the  $\sim 0.15$  observed here. Since critical,  $O(4)$  behavior results from self-interaction among the four light modes, the interaction of the four light modes with these nonuniversal, nearly degenerate states is expected to alter this behavior. Thus, our results suggest that  $O(4)$  critical behavior

should not be seen in  $N_t = 4$  thermodynamics at least for  $|\beta - \beta_c| \approx 0.03$ .

In conclusion, we have numerically studied anomalous symmetry breaking by examining quantities whose anomalous behavior comes directly from infrared effects. Given the relatively coarse lattice spacing in our simulations  $a \approx 1/3$  Fermi, our failure to find such effects above the 15% level is far from conclusive evidence that such effects are suppressed in nature [14]. However, this represents a first step in a systematic lattice calculation of such phenomena and must be followed by more demanding calculations on finer lattices and calculations using fermion formulations with improved chiral properties.

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