Search for a parity-flavor-breaking phase in QCD with two flavors of Wilson fermions for $\beta \ge 5.0$

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We present data testing the existence of a parity-flavor-breaking phase in simulations of QCD with two flavors of light Wilson fermions. This is done by explicit simulations on lattice sizes of 6^4 , 8^4 , and 10^4 for a variety of values of β and κ as well as the coefficient *h* of an explicit breaking term included in the action. We find that at $\beta = 6/g^2$ equal to or greater than 5.0 extrapolation in the parameter *h* as well as in the lattice volume show no indication of a phase where parity and flavor are spontaneously broken in the limit of zero *h*. [S0556-2821(97)03517-0]

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I. INTRODUCTION

For many years now, Aoki [1-5] and collaborators [7-9] have been advocating the existence of a parity-flavorbreaking phase in QCD with Wilson fermions as a means of explaining why the pion mass in this model approaches small values as the Wilson parameter κ approaches, for every value of inverse square coupling β , a critical value κ_c . This is in spite of no-go theorems [10,11] that forbid such a phase in the continuum limit.

Indeed analytic arguments have been presented to support the existence of such a phase at $\beta = 0.0$. For finite and, in particular, larger values of β where current lattice simulations are undertaken, such evidence is lacking [9].

Although the picture advocated by Aoki may explain the smallness of the pion masses as κ approaches κ_c it also explicitly states that these pions are not the Goldstone modes of spontaneous chiral symmetry breaking. This presents a problem in that it is then not clear that any of the soft pion and other theorems associated with this phenomenon will be respected on the lattice. In other words, this would not be the expected simulation of true QCD. In fact, the large N analytic analysis, which indicates the existence of this phase at $\beta = 0.0$, also shows the nonvanishing of the π - π scattering length which is contrary to the expected spontaneous chiral symmetry breaking of QCD. This is of course unimportant at $\beta = 0.0$ but is very important, if true, at the values of β where current simulations are performed.

The alternative picture where the explicit chiral symmetry-breaking Wilson term causes the (otherwise Goldstone) pions to acquire a small mass proportional to the lattice spacing does not have such a problem. Indeed, that all these extra effects would disappear as the lattice spacing is made smaller with the approach to the continuum limit was formally demonstrated some time ago [12,13,15].

Several models exhibit a parity-flavor-breaking phase. In the Nambu–Jona-Lasinio (NJL) [14,16,17] model with Wilson fermions this phase was numerically and, in the large N approximation, analytically [16,18] confirmed for values of β up to a specific cutoff value. This phase disappears for larger values of β . The Schwinger model with two flavors of Wilson fermions exhibits this phase at strong coupling and also loses it at weak coupling [19]. Whereas the picture advocated by Aoki does not anticipate such a quenching effect for the phase in QCD, recent phenomenological arguments by Creutz [20] tend to show a preference for quenching of this phase if it exists.

Thus it becomes necessary to explore this important feature by explicit simulations of QCD with Wilson fermions on volumes larger than those already studied [9].

II. SIGNATURE OF THE BROKEN PHASE

Following arguments presented by Aoki and Aoki and Gocksch [1,9], it is necessary, in order to investigate the presence of the parity-flavor-breaking phase in simulations, to introduce first an explicit breaking term into the action and then extrapolate the measured order parameter as this term tends to zero. Since the extrapolation is to be done, in principle, after the "infinite volume" limit is taken, such simulations must be done for larger volumes and any order parameter extrapolation be studied as a function of this increasing volume. In such a situation a typical behavior of the data at finite volumes that one might expect is shown in Fig. 1. It is expected that the functional dependence of the (measured) order parameter on h be such that for any *finite* volume this order parameter vanishes at h = 0.0.



FIG. 1. Expected variation of computed order parameter with volume.

TABLE I. Parameters and measured order parameter PF_L for the case of $\beta = 5.0$ on lattices of volume L^4 , for L = 6, 8, and 10.

к	h	PF_6	PF_8	PF_{10}
0.1500	0.001	0.01969(31)	0.01966(17)	0.01966(11)
0.1500	0.005	0.0983(15)	0.09834(86)	0.09835(51)
0.1500	0.050	0.968(15)		
0.1500	0.100	1.863(26)		
0.1500	0.300	4.310(48)		
0.1810	0.001	0.0259(20)	0.0277(22)	0.0273(2)
0.1810	0.005	0.1319(90)	0.1294(57)	0.1365(80)
0.1820	0.001	0.0255(17)	0.02629(98)	0.02559(8)
0.1820	0.005	0.1282(87)	0.1325(74)	0.1315(53)
0.1820	0.050	1.396(56)	1.389 (29)	
0.1820	0.100	2.382(56)	2.380 (32)	
0.1820	0.300	4.619(58)		
0.1850	0.001	0.0250(13)	0.0250(7)	0.0251(5)
0.1850	0.005	0.1225(52)	0.1273(71)	0.1223(18)
0.1850	0.050	1.287(65)		
0.1875	0.001			
0.1875	0.005			

The variation of this dependence with increasing volume is crucial to the initial determination of the existence of a broken phase or its absence. The existence of a broken phase in the infinite volume limit is signaled by a flattening of this dependence for larger values of h and a sharper drop to zero as h approaches zero. Thus it is clear that a significant volume dependence of the order parameter at smaller values of h is a necessary indicative factor for this phase. If, on the other hand, the approach to zero is not varying significantly as the volume increases, the infinite volume limit will not sustain a broken phase.¹

III. NUMERICAL SIMULATIONS

We report here on simulations done with two flavors of Wilson fermions at $\beta = 5.0$, 5.5, and 8.0 on volumes of 6^4 , 8^4 , and 10^4 for a variety of values of κ ranging from less than the appropriate κ_c to values greater than κ_c .

The choice of these three values of β was determined as follows. The value $\beta = 5.5$ represents current simulations on larger lattices where spectrum and matrix element calculations are being done; that at $\beta = 5.0$ represents a lower value below which relevance to continuum physics is not expected, and the last value at $\beta = 8.0$ is to extend the search to a much



FIG. 2. (a) Histogram of computed *PF* at β =5.0, κ =0.15, h=0.001 for all volumes considered; and (b) histogram of computed *PF* at β =5.0, κ =0.185, h=0.005 for all volumes considered.

larger value of β in case the parity-flavor-breaking phase were to be confirmed at the two smaller values.

We introduce into the QCD action a term of the form $ih\bar{\psi}\gamma_5\tau_3\psi$ where τ_3 is a 2×2 matrix representing the third element of the generators of flavor SU(2) algebra. Upon integrating the fermionic variables this is reflected in the simulation by the product of two determinants: DetM(h)*DetM(-h) where M(h) is given by a simple modification of the Wilson matrix M_W as

$$M(h) = M_W + ih\gamma_5$$
.

As pointed out by Aoki, we also have here

$$\gamma_5 M(-h) \gamma_5 = M^{\dagger}$$

and

$$\operatorname{Det} M(-h) = \operatorname{Det} M^{\dagger}(h).$$

Simulations were done for the parameter *h* taking values ranging from 0.001 to 0.3. For the volume dependence we concentrate on the smaller values of *h* and in particular h=0.001 and h=0.005 for all three volumes considered and mostly for values of κ greater than κ_c .

¹If not careful, one may arrive at wrong conclusions. If simulations are done only at larger values of h one may use the slightly varying values of the order parameter there to extrapolate these to *infinite volume*. If this step is then followed by a linear extrapolation to h = 0.0 a nonzero value for the order parameter at h = 0.0 may be obtained. At this stage it is tempting to conclude that a broken phase exists in that limit. This may be the wrong conclusion if this is not accompanied by a significant increase in the value of the order parameter at smaller values of h.



FIG. 3. (a) *PF* vs 1/*L* for β =5.0, κ =0.182, *h*=0.001; (b) *PF* vs 1/*L* for β =5.0, κ =0.182, *h*=0.005; (c) *PF* vs 1/*L* for β =5.0, κ =0.185, *h*=0.001; and (d) *PF* vs 1/*L* for β =5.0, κ =0.185, *h*=0.005.

The order parameter we compute is the expectation value of the operator $i\overline{\psi}\gamma_5\tau_3\psi$. With our notation this is given as

$$PF = -\operatorname{Im} \operatorname{Tr}(\gamma_5 M^{-1}(h)).$$

IV. RESULTS

For the three values of β considered, simulations were performed, as mentioned above, at various values of κ both below and above κ_c . We shall present the data and results for each value of β considered separately.

In all cases these simulations were also done at various values of the external parameter h. For each κ the results of the computions on the three volumes L^4 , L=6, 8, and 10, were compared at the two values of h=0.001, and h=0.005. The variation of the order parameter with 1/L is then used to obtain an "infinite volume" limit for all values of h used. The choice of 1/L is indicated here by the naive dimension of the order parameter. Following this, the order parameter at these values of h were fitted to

$$PF = A + Bh^{1/3} + Ch + Dh^2.$$

A separate fit to the pure quadratic polynomial

$$PF = A + Ch + Dh^2$$

was also done.

The initial aim in this case is to detect the possible existence of any nonzero constant *A* at h=0.0 as the limit of the order parameter at that point. This is of particular interest for comparing results at values of κ above κ_c with those below κ_c .

It is useful to point out here that in the presence of a parity-flavor-breaking phase the order parameter is expected to vary with h as

$$PF_{\infty} = A + Bh^{1/3} + \cdots$$

this being the behavior of the root of the cubic equation determining the position of the minimum of the quartic effective potential. In the absence of such a phase the same behavior follows with A = 0.0. As the quartic potential becomes quadratic, the leading behavior becomes

$$PF = Ch + \cdots$$
.

This should, when compared to the data, be also a useful tool in determining which situation one is in.



FIG. 4. (a) *PF* vs *h* for $\beta = 5.0$, $\kappa = 0.15$, and a quadratic fit; and (b) *PF* vs *h* for $\beta = 5.0$, $\kappa = 0.182$, and a quadratic fit.

TABLE II. Parameters and measured order parameter PF_L for the case of $\beta = 5.5$ on lattices of volume L^4 , for L = 6,8,10.

κ	h	PF_6	PF ₈	PF_{10}
0.1300	0.001	0.01689(22)		
0.1300	0.005	0.0844(10)		
0.1300	0.050	0.836(10)		
0.1300	0.100	1.633(20)		
0.1350	0.001	0.01750(23)	0.01750(14)	
0.1350	0.005	0.0874(12)	0.0875(7)	
0.1425	0.001	0.01860(29)	0.01863(17)	
0.1425	0.005	0.0931(15)		
0.1500	0.001	0.02000(40)	0.02009(24)	
0.1500	0.005	0.0998(20)		
0.1550	0.001	0.02079(51)	0.02140(36)	
0.1550	0.005	0.1039(26)		
0.1620	0.001	0.02132(54)	0.02200(42)	0.02246(31)
0.1620	0.005	0.1068(26)	0.1102(20)	0.1114(17)
0.1620	0.050	1.041(24)	1.052(14)	
0.1620	0.100	1.954(36)	1.969(22)	
0.1650	0.001	0.02158(6)	0.02205(43)	0.02299(29)
0.1650	0.005	0.1086(34)	0.1101(20)	0.1110(15)
0.1650	0.050	1.047(23)	1.056(14)	. /
0.1650	0.100	1.966(35)	1.984(21)	
0.1650	0.300	4.354(50)		



FIG. 5. Variation of *PF* with κ at $\beta = 5.5$ and h = 0.001.

A. $\beta = 5.0$

The value of κ_c at this value of β is known to be about 0.18. We, consequently, performed simulations well below that value at $\kappa = 0.15$ and well above it at $\kappa = 0.1875$ and intermediate values in between. We present in Table I the results of these simulations.

The results in Table I clearly show also that the values computed for the order parameter at the larger values of the volume are only incrementally different from those measured



FIG. 6. (a) *PF* vs 1/*L* for $\beta = 5.5$, $\kappa = 0.162$, h = 0.001; and (b) *PF* vs 1/*L* for $\beta = 5.5$, $\kappa = 0.162$, h = 0.005.



FIG. 7. (a) *PF* vs *h* for β =5.5, κ =0.162, and a quadratic fit; and (b) *PF* vs *h* for β =5.5, κ =0.165, and a quadratic fit.

on the small volume for all values of κ indicated. For values of κ less than κ_c , these results are consistent within errors. This is best illustrated by the overlapping histograms of these measurements at $\kappa = 0.15$ given in Fig. 2(a). For $\kappa = 0.185$ a similar histogram, Fig. 2(b), indicates only an incremental increase of the peak of the distribution with volume. This incremental change may be used to obtain an "infinite volume limit" of these values assuming a linear extrapolation in 1/L where L is the lattice linear dimension as shown, for example, in Figs. 3(a)-3(d). It is clear here that the data are consistent with being essentially "constant" with volume. A quadratic fit in h to this "infinite volume values" is not significantly different from a fit to the data at volume 6^4 where we obtain, for example, Figs. 4(a) and 4(b), a zero constant for the extrapolated value of the order parameter at h=0.0 for $\kappa=0.15$ below κ_c and $\kappa=0.182$ slightly above it. For values of κ both below and above κ_c this clearly implies the absence of any volume dependence of the order parameter and, hence, in both cases and in particular the latter case, the absence of a parity-flavor-breaking phase in the system at $\beta = 5.0$. A fit with a leading $h^{1/3}$ is not as good a description of the data as it leads to a much higher χ^2 . Hence, we further conclude that the effective potential of the system is predominanty quadratic at small h.

<u>56</u>

TABLE III. Parameters and measured order parameter PF_L for the case of $\beta = 8.0$ on lattices of volume L^4 , with L = 6,8,10.

к	h	PF ₆	PF_8	PF_{10}
0.1200	0.001	0.01591(19)		
0.1200	0.005	0.0796(10)		
0.1200	0.050	0.7845(89)		
0.1200	0.100	1.541(17)		
0.1300	0.001	0.01691(25)	0.01708(15)	0.01702(10)
0.1300	0.005	0.0843(12)	0.0851(7)	0.0851(7)
0.1300	0.050	0.832(10)		
0.1300	0.100	1.627(19)		
0.1400	0.001	0.01782(29)		
0.1400	0.005	0.0897(18)		
0.1400	0.050	0.875(14)		
0.1400	0.100	1.732(22)		
0.1460	0.001	0.01806(30)	0.01861(20)	0.01853(14)
0.1460	0.005	0.0908(16)	0.0926(12)	0.0927(7)
0.1460	0.050	0.892(14)		
0.1460	0.100	1.721(25)		
0.1500	0.001	0.01823(29)	0.01857(21)	0.01855(10)
0.1500	0.005	0.0920(17)	0.0928(9)	0.0927(6)
0.1500	0.050	0.902(14)		
0.1500	0.100	1.736(26)		
0.1550	0.001	0.01838(29)		
0.1550	0.005	0.0919(15)		
0.1600	0.001	0.01829(28)		
0.1600	0.005	0.0921(15)		
0.1600	0.050	0.905(13)		
0.1600	0.100	1.749(25)		
0.1800	0.001	0.02012(76)		
0.1800	0.005	0.0896(12)		
0.1800	0.050	0.878(13)		
0.1800	0.100	1.703(22)		

B. $\beta = 5.5$

The value of κ_c in this case is also known to be in the neighborhood of $\kappa = 0.16$. Table II details the results of our computations for values of κ well below and above this value. We concentrate in this discussion on the results obtained at $\kappa = 0.162$ and 0.165, both above κ_c and where the postulated phase is expected to exist.

We show in Fig. 5 the variation of the computed order parameter with κ over the range used for h = 0.001. No sharp change is indicated as the value of $\kappa_c = 0.16$ is crossed.

Analysis similar to that described above is also performed for this data set.

The results at the larger volumes show only an incremental increase, if any, as shown, for example, for the case of $\kappa = 0.162$ at both h = 0.001 and h = 0.005, in Figs. 6(a) and 6(b).

Here again an "infinite volume" limit may indeed be inferred and a quadratic fit in h gives for the "constant" in the fit a value which is consistent with zero as shown in Figs.

0.12



FIG. 8. Variation of *PF* with κ at $\beta = 8.0$ and h = 0.005.

7(a), and 7(b) for $\kappa = 0.162$ and $\kappa = 0.165$.

We are then again led to conclude the absence of a parity-flavor-breaking phase at these values of κ above κ_c .

Attempts at fits with a leading $h^{1/3}$ behavior again lead invariably to worse fits indicating again a dominant quadratic behavior of the effective potential for the order parameter.



FIG. 9. (a) *PF* vs 1/*L* for β =8.0, κ =0.146, *h*=0.005; and (b) histogram of computed *PF* at β =8.0, κ =0.15, *h*=0.005 for all volumes considered.



FIG. 10. (a) *PF* vs *h* for β =8.0, κ =0.146, and a quadratic fit; and (b) *PF* vs *h* for β =8.0, κ =0.16, and a quadratic fit.

C. $\beta = 8.0$

The value of κ_c in this case has not been determined numerically. We estimate its value using a tadpole improved perturbative procedure as discussed in [21]. We obtain in this case a value in the neighborhood of $\kappa_c \approx 0.145$. Consequently, our simulations are performed at values of κ below and above this value as shown in Table III.

We show in Fig. 8 the variation of the computed order parameter with κ over the range used. No sharp change is indicated as the value of $\kappa_c \approx 0.145$ is crossed.

We concentrate here on the data at the values of κ above κ_c . Using the same procedure as above, essentially the same conclusion follows. Figures 9(a) and 9(b) show that no significant change in the evaluation of the order parameter at the larger volumes exists for $\kappa = 0.146$ at h = 0.005 and as seen by the overlapping histograms for $\kappa = 0.15$ at h = 0.005.

Furthermore, quadratic fits in *h* at, for example, $\kappa = 0.146$ and $\kappa = 0.16$ again have a leading "constant" that is consistent with zero as shown in Figs. 10(a) and 10(b), respectively. Therefore, one is led again to the absence of any signal for a parity-flavor-breaking phase at this value of β .

Finally the obvious leading linear dependence of the fit indicates again a dominant quadratic effective potential at this value of β as well.

It is clear from the discussion above that, up to lattice volumes of 10^4 , simulations of QCD with two flavors of Wilson fermions do not indicate a parity-flavor-breaking phase at $\beta \ge 5.0$ as postulated by Aoki and collaborators.

The authors of Ref. [6] argue, however, that such signals may only be seen at larger volumes for larger values of β , in such a way that one needs to be at infinite volume in the weak coupling limit. This possibility is based on the behavior that actually happens for the two-dimensional Gross-Neveu model.

This of course need not happen for QCD, but the possibility should be considered. Unfortunately, it is not subject to total elimination through finite volume simulations. This is so as the arguments of [6] supporting a volume dependence of the signal requires at least one dimension of the lattice to be already large (infinite) in extent. Clearly, if a signal is not seen for a prechosen large volume one might always argue that it happens yet at a larger volume than the one used.

An alternative possibility is represented by the Nambu– Jona-Lassinio model in four dimensions, which also exhibits a parity-flavor-breaking phase for small values of β . This model does not exhibit such a phase above a cutoff value of β even for infinite volume as shown in [18,16,17]. The phase region pinches out at a finite value of β .

Thus, whereas our results do not indicate that a nonzero value of *PF* at h=0 emerges for $\beta \ge 5.0$ for lattice sizes up

to 10⁴, we are not in a position to exclude the possibility that such a signal (for the existence of a parity-flavor-broken phase) may emerge for lattice sizes that are larger than 10⁴. It has been demonstrated that at $\beta = 0.0$ such a phase may exist in QCD in the large N (color) limit. It has also been demonstrated using various volumes that this phase does extend beyond $\beta = 0.0$ at least up to $\beta = 3.5$. Should the analogy with the NJL model hold, this phase could pinch out at a $\beta < 5.0$. Our data, up to the volumes considered (10⁴), favor this alternative.

It should be remarked that all current fits to spectrum and current matrix element computations done near κ_c and at volumes up to $16^3 \times 32$ rely on the chiral Goldstone nature of the pions. Indications, therefore, are such that, as shown formally sometime ago, the behavior of QCD in this region is simply related to the approach to zero lattice spacing and infinite volume of a theory that is fundamentally with a Goldstone chiral realization as QCD is expected to be.

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