Metastabilities in Three-Flavor QCD at Low Quark Masses

R. V. Gavai
Tata Institute of Fundamental Research, Bombay 400005, India

and

J. Potvin and S. Sanielevici
Physics Department, Brookhaven National Laboratory, Upton, New York 11973
(Received 4 March 1987)

Using a Langevin algorithm to incorporate low-mass dynamical quarks, we simulate QCD with three light flavors on an $8^3\times4$ lattice. We find clear metastabilities in lattice measurables at a quark mass of 0.025 in lattice units, whereas earlier analyses at 4 times the mass above did not prove their presence. Our results suggests a first-order chiral phase transition in three-flavor QCD. We also confirm the presence of a stronger first-order transition with four flavors and indicate the possibility of a weaker first-order transition with two flavors.

PACS numbers: 12.38.Gc, 11.30.Rd, 12.38.Aw, 12.38.Mh

Numerical simulations of lattice quantum chromodynamics (QCD) at finite temperature have provided us with important information for the forthcoming relativistic-heavy-ion collision experiments. Whereas a variety of issues, such as the proper incorporation of dynamical quarks, are still far from settled, one property of hot QCD seems to show up in all the works so far: The energy density jumps rather sharply by about an order of magnitude in a very small interval of temperature. Whether this abrupt change is due to a first-order phase transition has been a subject of intense activity in the recent past.[1] This question is clearly very important for an understanding of the general properties of strongly interacting matter, in particular the experimental signatures of the quark-gluon plasma.

By extracting the relevant symmetries from QCD, one can write down models which can be treated analytically to yield predictions for the deconfinement[2] phase transition and for the chiral-symmetry-restoring[3] phase transition in QCD. Such considerations lead one to expect that QCD with three flavors should have a first-order deconfinement transition for infinitely heavy quarks and a first-order chiral phase transition for massless quarks. As one approaches the physical quark masses from either of the two limits, one expects a progressively weaker first-order phase transition with decreasing latent heat. By the methods of Ref. 3, the chiral transition is predicted to be first order for $n_f \geq 3$ continuum flavors while no prediction could be made for $n_f = 2$.

It is a major challenge for numerical simulations to verify these predictions and to improve upon them. The existence of a first-order deconfinement transition in pure SU(3) theory is solidly established.[1] The problem is to determine the order of the chiral transition with the same degree of confidence. Two groups[4,5] have studied lattice QCD with three light dynamical flavors. Both employed staggered fermions and used a prescription proposed by Hamber *et al.*[6] to simulate three continuum flavors. This prescription is motivated by perturbative arguments and is widely used although its validity away from the continuum limit is not yet rigorously proved. Using the pseudofermion method[7] to include the dynamical quarks these authors simulated QCD with a quark mass $ma = 0.1$ (in lattice units) on $8^3\times4$ and $6^3\times4$ lattices. While their results showed substantial quantitative agreement, they differed on the order of the phase transition. It thus appears that the transition is at best very weakly first order at $ma = 0.1$. Similar conclusions were also reached for the four-flavor case[8] where various fermion algorithms were used. Gupta *et al.*[9] have simulated QCD with four flavors using a direct computation of the fermion determinant on a 4^4 lattice. They find that, by reducing the mass to $ma = 0.025$, one obtains clear metastability signals for the average plaquette, for the real part of the Wilson line, and for the chiral order parameter.

One immediately wonders whether a similar situation occurs in three-flavor QCD—namely, whether the transition becomes a lot sharper when the mass is reduced fourfold. One would also like to check whether the phenomenon is, perhaps, only an artifact of the small symmetric lattice. The fact that their algorithm is very expensive makes it difficult to answer the latter question. We have, therefore, used a much faster method and found that it is as reliable as the direct algorithm in investigating the order of the phase transitions under discussion. After confirming the findings of Ref. 9, we proceeded to study three-flavor QCD on 4^4 and $8^3\times4$ lattices. We do find clear metastabilities for both lattice sizes. The signal on the larger, asymmetric lattice is much clearer. Finally, we studied the two-flavor case on the 4^4 lattice and found possible indications of a weak metastability signal.

We use the discrete first-order Langevin algorithm described by Gavai, Potvin, and Sanielevici.[10] To simulate n_f continuum flavors by means of staggered lattice fermions, we use the prescription of Ref. 6 alluded to above. The boundary conditions are periodic in the space directions and antiperiodic in the time direction. Because the Langevin time step is finite, $\epsilon \neq 0$, such an algorithm converges to an equilibrium action which differs from the action of lattice QCD at color coupling $\beta = 6/g^2$ with n_f quark flavors.[10] The difference between the two actions can be expanded in powers of ϵ. A major effect of the first-order error is a shift in β, n_f, and the quark mass m: The "true values" of these parameters are, to first order in ϵ, $\bar{\beta} = \beta[1 - \epsilon(C_F - C_A)/12]$; $\bar{n}_f = n_f(1 - \epsilon C_A/12)$; $\bar{m} = m(1 - \epsilon C_F/4)^{-1}$. C_A and C_F in these formulas denote the Casimar invariants in the adjacent and fundamental representations of SU(3), respectively.

Our investigation[10] has shown that higher-order systematic errors are not negligible with respect to the first-order errors unless ϵ is small. However, one can still hope that the equilibrium action of the Langevin process has the same thermal phase structure as lattice QCD. Of course, one must expect additional shifts arising from the analytically unknown higher-order error terms. In particular, one should not place quantitative confidence in values of phase transition couplings measured by the Langevin method. To minimize such effects while keeping the algorithm as efficient as possible, we have calculated with $\epsilon = 0.01$ and used the first-order compensation formulae to determine the updating parameters β, n_f, and m which correspond to the "physical values" $\bar{\beta}$, $\bar{n}_f$, and $\bar{m}$ at which we wish to run.

The inversion of the fermion matrix, required in the algorithm we use, was done by the conjugate gradient (CG) method. We found that a residue $r = 0.02$ (in the normalization of Ref. 10) is reached in about 200 CG iterations on an average configuration in the random phase and in about 80 iterations in the ordered phase. We have also tried $r = 0.005$ and found essentially the same results for the measured observables. Imposing a limit of 90 CG iterations, as in Ref. 9, also led to very similar results.

In preliminary investigation, we checked that our method is able to detect the well-known first-order deconfining transition in pure SU(3), even on the small symmetric 4^4 lattice. We then proceeded to simulate QCD with staggered dynamical quarks of mass $\bar{m}a = 0.025$ on the 4^4 lattice. Figure 1 presents the results in terms of run-time histories of the 1×1 Wilson

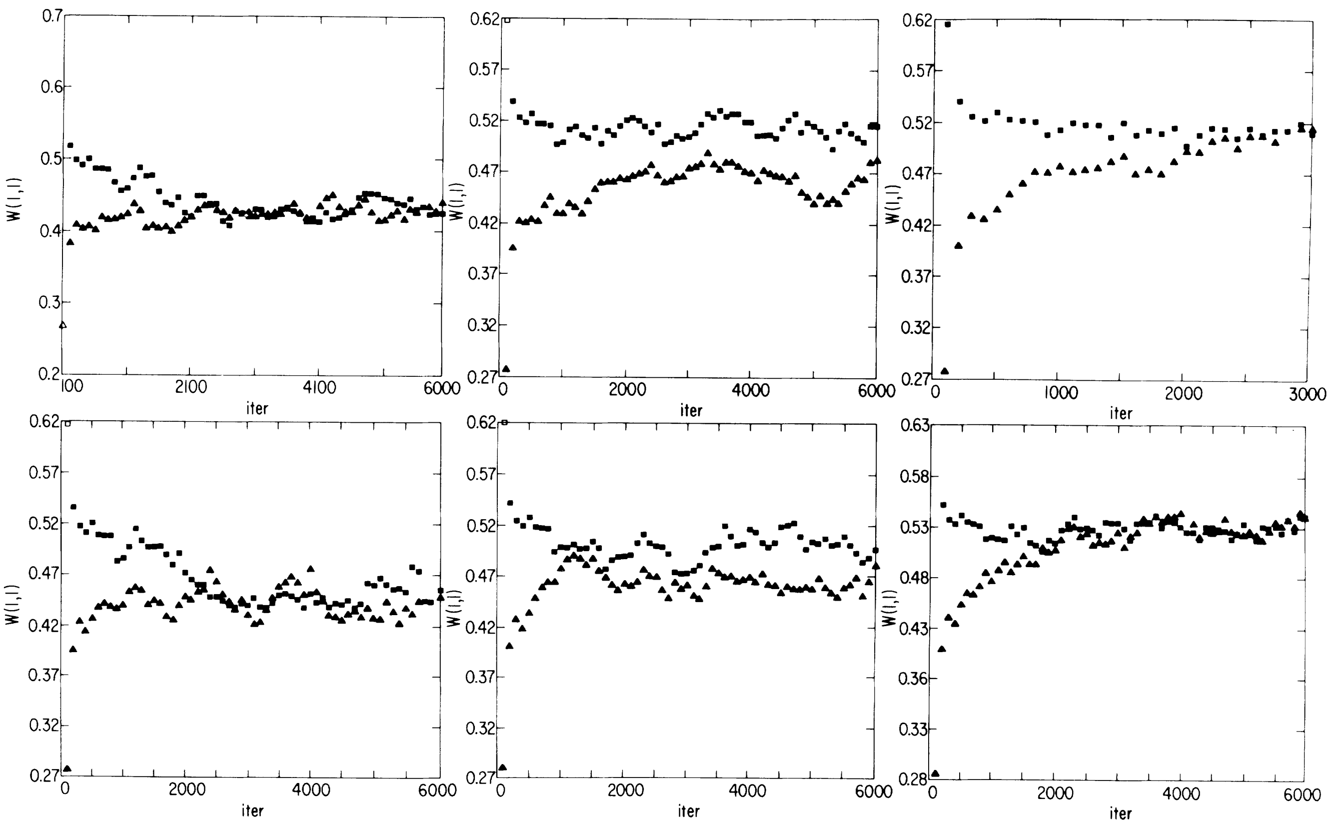

FIG. 1. Time histories for the 1×1 Wilson loop in QCD with four and three continuum flavors of quarks of mass $\bar{m}a = 0.025$ on a 4^4 lattice. Upper row: $\bar{n}_f = 4$, $\bar{\beta} = 5.0$, 5.03, 5.1 from left to right. Lower row: $\bar{n}_f = 3$, $\bar{\beta} = 5.05$, 5.1, 5.2 from left to right. Squares describe the runs from disordered starts and triangles describe the runs from ordered starts. Each point represents the naive average over 100 iterations. All runs use $\epsilon = 0.01$.

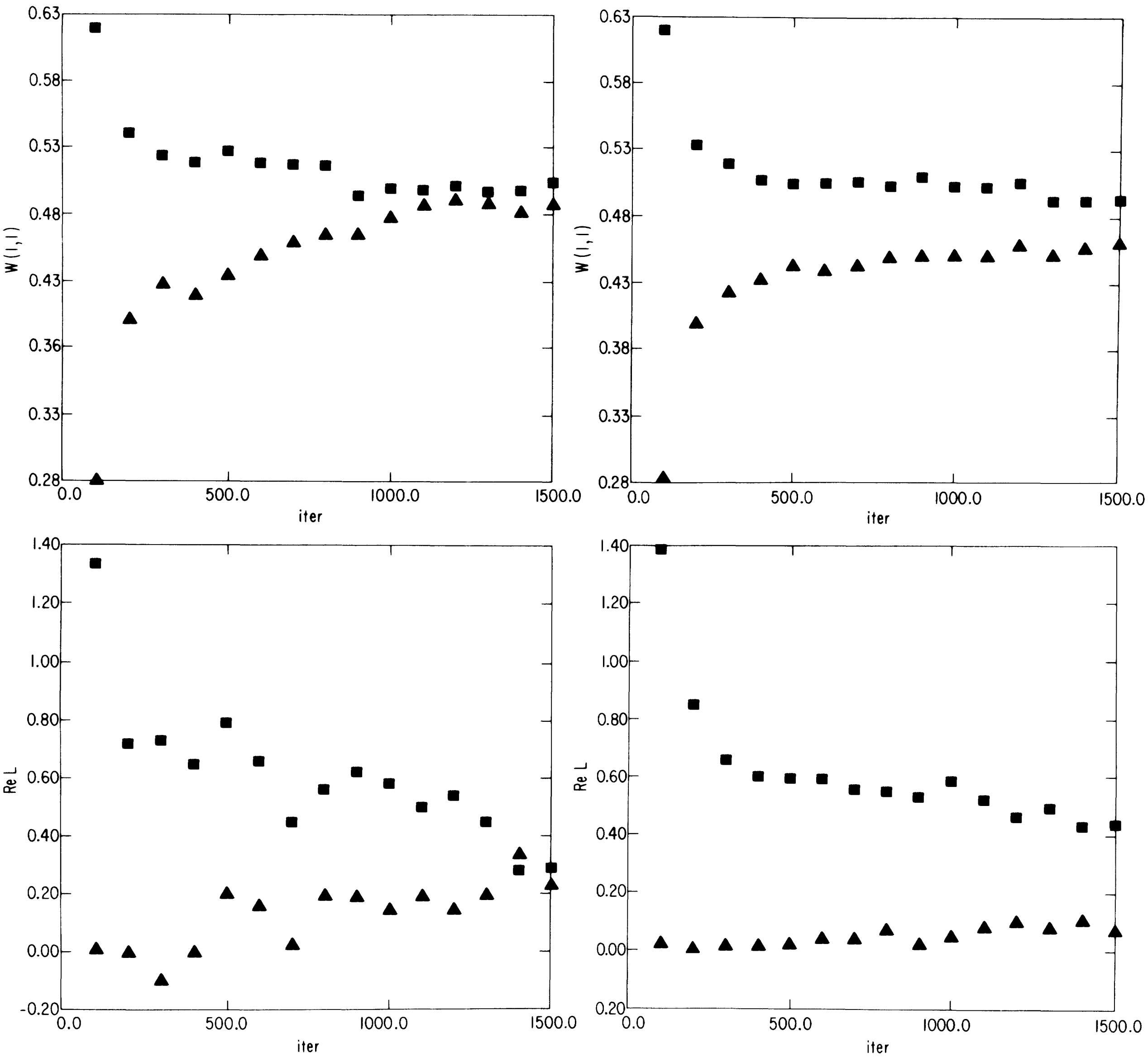

FIG. 2. Metastability signals in three-flavor QCD on a 4^4 and on an $8^3 \times 4$ lattice ($\overline{m}a = 0.025$). $\epsilon = 0.01$, $\bar{n}_f = 3$, $\bar{\beta} = 5.1$. The upper row shows the 1×1 Wilson loop $W(1,1)$ and the lower row shows the real part of the thermal Wilson line ReL. The run at left was on a 4^4 lattice and the run at right on an $8^3 \times 4$ lattice. Note that ReL as plotted differs from the usual normalization by a factor of 3.

loop $W(1,1)$. We see that 6000 (and even 3000) iterations are sufficient to distinguish whether the theory is in its disordered or in its ordered phase or in the transition region. Since we are not interested in measuring absolute average values of lattice quantities, we are not hampered by correlations between measurements.

For $\bar{n}_f = 4$ the metastability signal around $\bar{\beta} = 5.03$ appears very clear even compared to the sizable finite-size fluctuations. We can thus confirm the result of Ref. 9. The fact that our critical coupling differs from theirs ($\beta = 4.9$) is surely due in part to the first-order character of our compensation formulas, as noted above. On the other hand, because of the expensive nature of their algorithm, Gupta *et al.* were not able to search for the exact location of the phase transition. It is conceivable that their signal would become more pronounced at higher β, closer to our value.

For $\bar{n}_f = 3$, we note that the transition has shifted to $\bar{\beta} \approx 5.1$ and that the metastability signal (the gap between the coexistent equilibria) appears weaker with respect to the finite-size fluctuations. Figure 2 compares the first 1500 iterations on the 4^4 lattice at $\bar{\beta} = 5.1$ to those on an $8^3\times4$ lattice at the same $\bar{\beta}$. The enhancement of the signal-to-noise ratio by going to the larger lattice is quite impressive and strongly suggests that the chiral transition in three-flavor QCD is indeed of first order. Further data are currently being gathered on the $8^3\times4$ lattice.

We have also investigated the two-flavor case on the 4^4 lattice. We found that the phase transition occurs around $\bar{\beta}=5.33$ but that 3000 iterations on the small lattice cannot discriminate between a possible weak metastability signal and a rapid crossover. It seems reasonable to hope that the order of the transition can be conclusively established on the $8^3\times4$ lattice.

To conclude, we have shown that three-flavor QCD has metastabilities at quark mass 0.025 on a 4^4 and an $8^3\times4$ lattice. With our Langevin simulation method, we have confirmed a similar finding obtained for four flavors on a 4^4 lattice with a different algorithm.[9] Combined with the earlier results at mass 0.1, our results support the prediction of Pisarski and Wilzcek[3] that the chiral transition should be first order for QCD with three or more massless flavors and that this transition progressively weakens as m is increased. Our simulations suggest that the first-order character of the transition also weakens progressively as the number of flavors is decreased from four to three to two, the mass being held constant. The interval in β at which the transition occurs is found, as expected, to shift upwards as the number of flavors is decreased.

After completion of this manuscript, we learned that the findings of Ref. 9 have also been confirmed with use of the hybrid algorithm.[11]

It is a pleasure to thank Mike Creutz for helpful discussions. The computations were done on the Cray X-MP at the National Magnetic Fusion Energy Computer Center, Livermore. This work was supported by the U.S. Department of Energy under Contract No. DE-AC02-76CH00016.

[1]J. Cleymans, R. V. Gavai, and E. Suhonen, Phys. Rep. **130**, 217 (1986); R. V. Gavai, in *Intersections between Particle and Nuclear Physics—1986*, edited by D. F. Geesaman, AIP Conference Proceedings No. 150 (American Institute of Physics, New York, 1987).

[2]B. Svetitsky, Phys. Rep. **132**, 1 (1986).

[3]R. D. Pisarski and F. Wilczek, Phys. Rev. D **29**, 338 (1984).

[4]F. Fucito, C. Rebbi, and S. Solomon, Nucl. Phys. **B180 [FS2]**, 615 (1984), and Phys. Rev. D **31**, 1461 (1985); F. Fucito and S. Solomon, Phys. Rev. Lett. **55**, 2641 (1985).

[5]R. V. Gavai and F. Karsch, Nucl. Phys. **B261**, 273 (1985).

[6]H. W. Hamber, E. Marinari, G. Parisi, and C. Rebbi, Phys. Lett. **124B**, 99 (1983).

[7]F. Fucito, E. Marinari, G. Parisi, and C. Rebbi, Nucl. Phys. **B180 [FS2]**, 369 (1981).

[8]R. V. Gavai, Nucl. Phys. **B269**, 530 (1986), and references therein; M. Fukugita and A. Ukawa, Phys. Rev. Lett. **57**, 503 (1986); J. B. Kogut and D. K. Sinclair, Illinois University, Urbana Report No. ILL-(TH)-86-46, 1986 (to be published).

[9]R. Gupta, G. Guralnik, G. W. Kilcup, A. Patel, and S. R. Sharpe, Phys. Rev. Lett. **57**, 2621 (1986).

[10]R. V. Gavai, J. Potvin, and S. Sanielevici, Phys. Lett. **183B**, 86 (1987), and Brookhaven National Laboratory Report No. BNL-39021/TIFR/TH/86-38, 1986 (to be published), and references therein.

[11]J. B. Kogut, H. W. Wyld, F. Karsch, and D. K. Sinclair, University of Illinois, Urbana, Report No. ILL-(TH)-87-6, 1987 (to be published); E. V. E. Kovacs, D. K. Sinclair, and J. B. Kogut, Phys. Rev. Lett. **58**, 751 (1987).