Numerical determination of the QCD [beta] function

Gavai, R. V.; Karsch, Frithjof

Numerical Determination of the QCD β Function

R. V. Gavai
Physics Department, Brookhaven National Laboratory, Upton, New York 11973

and

F. Karsch
Physics Department, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801
(Received 18 March 1986)

The β function of SU(3) lattice gauge theory with three flavors of light dynamical quarks is obtained numerically by use of the (improved) ratio method. It appears to have a dip structure similar to that found in the theory without quarks. Our data seem to suggest that deviations from asymptotic scaling may be small for $\beta \gtrsim 5.3$.

PACS numbers: 12.38.Gc

Monte Carlo simulation of quantum field theories, formulated on the lattice, has now become the most important nonperturbative technique which one can use to obtain quantities such as hadronic masses from the underlying theory. An important step in such calculations is the continuum limit which consists of removal of the lattice regularization by taking the limit of vanishing lattice spacing a. The physical predictions should be independent of the cutoff. The β function of the theory tells us how to tune the bare coupling constant in the continuum limit so as to obtain the physical predictions. It is thus important to uncover and understand the structure of the β function of a theory. Recently a lot of effort has therefore been devoted to investigations of (nonperturbative) determinations of the β function for SU(2) and SU(3) gauge theories.[1] Two different methods have been employed so far: (i) the Monte Carlo renormalization-group (MCRG) method[2] and (ii) the ratio method.[3,4] The former combines the real-space renormalization-group approach with Monte Carlo simulation, whereas the latter involves a comparison of Wilson loops which differ in size by a factor of 2. In the case of a theory with dynamical fermions, such as QCD, a straightforward application of the MCRG method is made difficult by the Grassmannian nature of the fermion variables. On the other hand, the ratio method can still be used,[5] provided that gauge configurations incorporating the effects of dynamical fermions can be generated on the computer. A lot of different algorithms now exist which can achieve it fairly efficiently. While the field of development of such algorithms is still evolving rapidly, we feel that it has matured enough to allow us to extract the β function of QCD. Indeed, one can even perform a consistency check on the fermion algorithm by comparing the results with asymptotic-scaling predictions.

In this Letter, we report first results on the nonperturbative β function of QCD with three light (dynamical) flavors. Using the staggered-fermion formalism and the pseudofermion algorithm, we simulated SU(3) lattice gauge theory (with Wilson action) with three light dynamical quarks. Measuring various Wilson loops on the configurations so generated, we obtained information on the β function by use of the ratio method. The method consists of forming basic ratios

$$R(i_1,i_2,j_1,j_2)=\frac{W(i_1,i_2)}{W(j_1,j_2)},$$
$$R(i_1,i_2,i_3,i_4,j_1,j_2,j_3,j_4)=\frac{W(i_1,i_2)W(i_3,i_4)}{W(j_1,j_2)W(j_3,j_4)}, \tag{1}$$

such that $i_1+i_2=j_1+j_2$ and $i_1+i_2+i_3+i_4=j_1+j_2+j_3+j_4$ in the two cases, respectively. As noticed by Creutz[6] already, these ratios are free from perturbative singularities, and they satisfy the homogeneous renormalization-group equations

$$R(2i_1,2i_2,2j_1,2j_2;\beta,L)=R(i_1,i_2,j_1,j_2;\beta',L/2),$$
$$R(2i_1,2i_2,2i_3,2i_4,2j_1,2j_2,2j_3,2j_4;\beta,L)=R(i_1,i_2,i_3,i_4,j_1,j_2,j_3,j_4;\beta',L/2). \tag{2}$$

$\Delta\beta(\beta)=\beta-\beta'$ is the change in the coupling required to compensate the change of scale of a factor of 2. The parameters L and $L/2$ denote the linear sizes of the lattices on which the ratios are calculated. When β' is tuned such that Eq. (2) is satisfied, then the lattice size in physical units occurring on both sides of the equation is same, ensuring minimum finite-size effects. Using the definition of the β function [denoted here by $B(g^2)$] one can easily show that $\Delta\beta$ defined above is related to it by

$$\int_{\beta-\Delta\beta}^{\beta}\frac{dx}{x^{3/2}B(6/\sqrt{x})}=-\frac{2\ln 2}{\sqrt{6}}, \tag{3}$$

where we have used the definition $\beta=6/g^2$ for QCD. For large β, or equivalently small g^2, the β function is

TABLE I. Summary of results for $\Delta\beta$ for SU(3) gauge theory with three light flavors, obtained by use of the basic ratios.

β	Cut	$\Delta\beta$	$(\Delta\beta)_{\min}$	$(\Delta\beta)_{\max}$
5.4	0.08	0.82	0.81	0.83
5.6	0.05	0.317	0.290	0.347
5.8	0.05	0.535	0.523	0.545
6.0	0.07	0.609	0.561	0.637
6.2	0.11	0.567	0.373	0.681

dominated by the two universal terms

$$B(g) = -\frac{33-2n_f}{48\pi^2}g^3 - \frac{153-19n_f}{384\pi^4}g^5 + O(g^7), \quad (4)$$

where n_f is the number of massless flavors. From Eqs. (3) and (4) one obtains that

$$\Delta\beta = 0.474 + 0.128/\beta + O(\beta^{-2}), \quad (5)$$

for $n_f = 3$ and sufficiently large β. An agreement with the prediction above would act as a check on our method of including the dynamical fermions in the numerical simulations. Noting that any linear combination of the ratios in Eq. (2) also satisfies the equation, one can define "improved" ratios from which lattice-artifact corrections are eliminated. We will use the tree-level improved ratios $R_{12} = R_1 + \alpha R_2$, where α is determined by the requirement that these artifacts cancel in tree-level perturbation theory[7] (i.e., by requiring $\Delta\beta = 0$).

Our results were obtained for $L = 8$ in Eq. (2) by measuring all Wilson loops up to size 6×6 on the 8^4 lattice and 3×3 on the 4^4 lattice. The bare mass for the fermions was chosen to be $ma = 0.1$ on the 8^4 lattice and 0.2 on the 4^4 lattice. This amounts to a neglect of the logarithmic corrections under the scale change of 2 due to anomalous dimensions. The effect of dynamical fermions was taken into account by performing fifty pseudofermion hits at an average acceptance level of $\sim 70\%$ in the gauge sector. From previous studies it is expected that these choices are fairly optimal. Wilson loops were measured over typically a few thousand iterations in each case, discarding a thousand for equilibration. The errors on the measurements have been corrected for sweep-to-sweep correlations. Tables I and II display the results for $\Delta\beta$ obtained from matching the basic ratios and the tree-level improved ratios, respectively. To obtain the precise value of β' a linear interpolation between the ratios measured at various different β' values has been used. Except for $\beta = 5.4$, about ten ratios were used in the first case and twenty in the second case to determine $\Delta\beta$. The magnitude of fluctuations at each β, and hence a naive estimate of error, can be obtained

TABLE II. Same as Table I, but obtained by use of tree-level improved ratios.

β	Cut	$\Delta\beta$	$(\Delta\beta)_{\min}$	$(\Delta\beta)_{\max}$
5.6	0.05	0.301	0.295	0.310
5.8	0.05	0.533	0.523	0.541
6.0	0.05	0.606	0.585	0.626
6.2	0.10	0.480	0.438	0.531

from the minimum and maximum values of $\Delta\beta$ given in the tables. Statistical fluctuations in the Wilson-loop values at $\beta = 5.4$, which themselves are quite small at low β, prevented us from obtaining more ratios at $\beta = 5.4$, and also the improved ratios at that β. Since the improvement is more relevant at high β, in Fig. 1 we have plotted the summary of our results by displaying the $\Delta\beta$ estimates from improved ratios except for $\beta = 5.4$. The errors shown here are more conservative; they correspond to the cuts used in the respective matching predictions. The dashed line is the prediction of Eq. (5).

Before we discuss the physical significance of Fig. 1, let us first make some simple observations based on it. One sees a clear dip structure in the $\Delta\beta$, which is rather similar to that observed in the theory without quarks but at a lower value of β. In the pure gauge theory the dip occurred[2-4] at $\beta = 6.0$, whereas we find a pronounced dip at $\beta = 5.6$ which seems to be some-

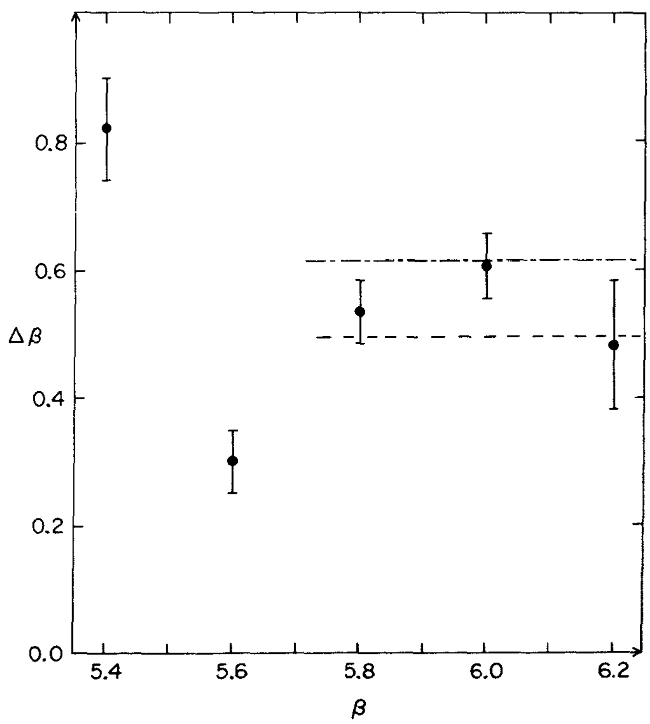

FIG. 1. $\Delta\beta$ as a function of β for QCD with three light dynamical flavors. The dashed line shows the asymptotic-scaling prediction of Eq. (5). Also shown above it is the asymptotic-scaling prediction for the quenched theory.

what narrower than the one in the pure gauge case: At $\beta = 5.4$ we observe already a large value of $\Delta\beta$ characteristic of the strong-coupling regime, and for $\beta > 5.8$ our data are consistent with the perturbative, asymptotic-scaling predictions. Thus, if we use the measured $\Delta\beta$ function of Fig. 1 as an input we conclude that across the dip the correlation length changes by a factor of 2, compared with the pure gauge theory where the dip covers a β range of 5.7 to 6.6, and the correlation length changes by a factor of about 4. Although the quality of our data is not very good, it does seem to suggest that unlike the theory without quarks the approach to asymptotic scaling may be again, from above, beyond the dip structure. Furthermore, the deviations from asymptotic scaling seem to be small for $\beta > 5.3$ (corresponding to $\Delta\beta \simeq 0.5$ at $\beta = 5.8$) compared to $\beta > 6.0$ in the pure SU(3) case. Bearing in mind the ongoing analysis of the scaling behavior of the pure SU(3) gauge theory, which still needs improvement and analysis on larger lattices and at larger β, it is clear that better data on larger lattices are necessary to confirm our findings and to clarify further the detailed structure of the β function of full QCD. In particular, since the difference between the asymptotic-scaling predictions of the quenched theory and the full theory is only 22% one may need estimates of $\Delta\beta$ with about one fifth the error of what we have in Fig. 1 in order to distinguish clearly between the two. We had typically 5000 iterations of the full theory at each β, and yet, as a result of the observed overshooting of the $\Delta\beta$ at $\beta = 6.0$, such a clear distinction was not possible. If the overshooting persists in a more detailed analysis, then the onset of asymptotic scaling might well be delayed until $\beta \simeq 5.7$.

The first analysis of the β function of full QCD presented here, however, clearly suggests a pronounced dip structure even in the presence of dynamical fermions. Of course, the structure of the dip, or even its presence, has no direct relevance to the practical calculations of, say, the hadron masses or the heavy quark potential. What would be relevant there would be the β at which asymptotic scaling sets in, which, as discussed above, may be at $\beta \simeq 5.3$. Nevertheless, in the general context of understanding how the theory goes over from the strong-coupling regime to the asymptotic-scaling regime and whether this crossover can be somehow smoothed by, say, modification of the action, it is interesting to note that the dip seems to be a more universal feature than previously thought. In the case of pure gauge theory the occurrence of the dip has been related[2,8] to the presence of a second-order phase transition in the fundamental-adjoint coupling plane. Monte Carlo data[9] seem to support this quantitatively. In the presence of dynamical fermions the number of flavors, n_f, introduces a new coupling in the effective action. One may now need to trace the phase diagram in this extended space of couplings to find out why it affects the β function of the full theory in approximately the same way as for $n_f = 0$. It has been argued that a nontrivial phase structure in the n_f-β plane appears with a second-order critical point for $(n_f, \beta) \sim (8, 4.67 \pm 0.1)$. $\Delta\beta(\beta)$ should have a zero at this point. For $n_f < 8$, it could lead to a dip structure in $\Delta\beta$ similar to the one observed in our simulations. In addition one would expect that the dip becomes deeper as n_f is increased to 8. Indeed, the data[10] for the scaling behavior of the chiral condensate in the $n_f = 4$ theory also suggest a narrow dip. It would be interesting to find a relation between the phase structure in the fundamental-adjoint plane of the pure gauge theory and the n_f-β plane of the theory with dynamical fermions. It may even be that the fermions act effectively as an adjoint gauge term in the action in addition to a renormalization of the fundamental coupling.

Finally, we exhibit in Fig. 2 our data on Wilson loops on the 8^4 lattice (at $\beta = 5.6$) along with that obtained in the pure SU(3) theory on a same size lattice

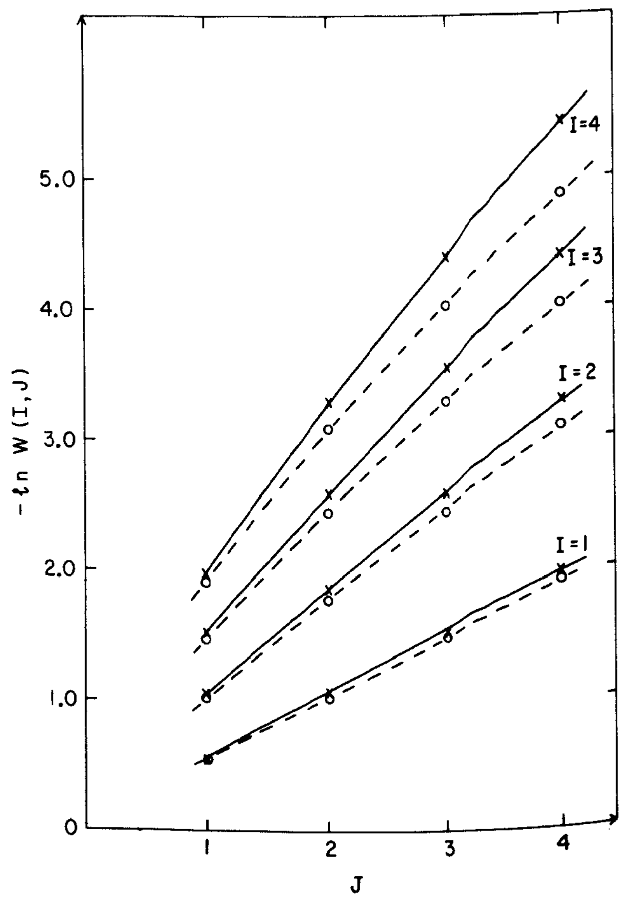

FIG. 2. $-\ln W(I,J)$ as a function of J for various I. The crosses show the pure SU(3) of Ref. 2 at $\beta = 5.8$ while the circles display our data at $\beta = 5.6$ for the theory with three light dynamical flavors. The error bars on all the points are smaller than or comparable to the size of the points themselves.

(at $\beta = 5.8$). The couplings have been so chosen that the plaquette value is about the same in both cases. The pure SU(3) data are well known to be consistent with a linear plus Coulomb term in the potential.[4,11] Pursuing the idea of such a potential in the full QCD, one naively expects screening to replace the confining linear term: $\sigma r \rightarrow (\sigma/\mu)(1-e^{-\mu r})$, with μ^{-1} as the screening length. Since $-\ln W$ directly measures the potential, and since the potential decreases faster in the full theory as r increases, one should see a systematic trend: The $-\ln W$ data for the full theory should always lie below corresponding pure SU(3) data, and the difference between the two should increase as the loop size grows. Figure 2 is in accord with this picture, lending one more support, albeit qualitative, to the fact that the pseudofermion method is able to include the fermion feedback correctly. Agreement of the data in Fig. 1 with the asymptotic-scaling prediction is a more quantitative check of this fact, although at present we have been able to check this at only the 1σ level.

To conclude, we have presented first results on the numerical, nonperturbative determination of the β function of QCD with three light flavors using the improved ratio method. The staggered-fermion formalism and the pseudofermion method were employed to simulate the full theory. Our results suggest a dip structure in $\Delta\beta$ that is analogous to the one seen in the quenched theory. Furthermore, our data seem to suggest that the deviations from asymptotic scaling may be rather small for $\beta \gtrsim 5.3$.

This work was supported by the U. S. Department of Energy under Contract No. DE-AC02-76CH00016 and by the National Science Foundation under Grant No. NSF-PHY-82-01948. The calculations reported here were done on the Cray computers at the National Magnetic Fusion Energy Computer Center, Livermore, and the National Center for Supercomputing Applications, University of Illinois, Urbana, whose support is gratefully acknowledged.

[1]F. Karsch, in *Proceedings of the Oregon Meeting*, edited by R. C. Hwa (World Scientific, Singapore, 1986); A. Patel and R. Gupta, in *Advances in Lattice Gauge Theory*, edited by D. W. Duke and J. F. Owens (World Scientific, Singapore, 1985), p. 206.

[2]R. Gupta, G. Guralnik, A. Patel, T. Warnock, and C. Zemach, Phys. Rev. Lett. **53**, 1721 (1984); R. Gupta *et al.*, Phys. Lett. **161B**, 352 (1985); K. C. Bowler, A. Hasenfratz, P. Hasenfratz, U. Heller, F. Karsch, R. D. Kenway, M. Meyer-Ortmanns, I. Montvay, G. S. Pawley, and D. J. Wallace, Nucl. Phys. **B257 [FS14]**, 155 (1985).

[3]A. Hasenfratz, P. Hasenfratz, U. Heller, and F. Karsch, Phys. Lett. **143B**, 193 (1984).

[4]K. C. Bowler, F. Gutbrod, P. Hasenfratz, U. Heller, F. Karsch, R. D. Kenway, I. Montvay, G. S. Pawley, J. Smit, and D. J. Wallace, Phys. Lett. **163B**, 367 (1985).

[5]U. Heller and F. Karsch, Phys. Rev. Lett. **54**, 1765 (1985).

[6]M. Creutz, Phys. Rev. D **23**, 1815 (1981); R. W. B. Ardill, M. Creutz, and K. J. M. Moriarty, Phys. Rev. D **27**, 1956 (1983).

[7]Note that in this order of perturbation theory the mixing coefficients α are independent of n_f; see, U. Heller and F. Karsch, Nucl. Phys. **B251 [FS13]**, 254 (1985).

[8]Yu. Makeenko and M. I. Polikarpov, Phys. Lett. **135B**, 133 (1984); G. Martinelli and M. I. Polikarpov, Yad. Fiz. **42**, 534 (1985) [Sov. J. Nucl. Phys. **42**, 337 (1985)].

[9]D. L. Chalmers, Phys. Lett. **160B**, 133 (1985).

[10]J. Kogut, University of Illinois Report No. ILL-(TH)-85-#81, 1985 (to be published).

[11]S. W. Otto and J. D. Stack, Phys. Rev. Lett. **52**, 2328 (1984).