PHYSICAL REVIEW D, VOLUME 61, 111501(R)

Finite density fat QCD

R. Aloisio,[1,4] V. Azcoiti,[2] G. Di Carlo,[3] A. Galante,[2] and A. F. Grillo[4]
[1] *Dipartimento di Fisica dell'Università dell'Aquila, L'Aquila 67100, Italy*
[2]*Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain*
[3]*Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali di Frascati, P.O.B. 13 - Frascati 00044, Italy*
[4]*Istituto Nazionale di Fisica Nucleare, Laboratori Nazionali del Gran Sasso, Assergi L'Aquila 67010, Italy*
(Received 3 March 1999; revised manuscript received 16 November 1999; published 19 April 2000)

Lattice formulation of finite baryon density QCD is problematic from the computer simulation point of view; it is well known that for light quark masses the reconstructed partition function fails to be positive in a wide region of parameter space. For a large bare quark mass, problems related to the phase of the determinant are still present but restricted to a small region in the chemical potential μ. We present evidence for a transition line that, starting from the temperature critical point at $\mu=0$, moves towards a smaller β with increasing μ.

PACS number(s): 12.38.Gc, 11.15.Ha

I. INTRODUCTION

From the point of view of computer simulations, the lattice approach to the nonperturbative aspects of quantum field theory is a mature technique; apart from a few exceptions, well consolidated schemes of simulation do exist that allow studies of the most interesting features of QCD. The ''few exceptions,'' however, concern very interesting problems as well. The most paradigmatic of these dark zones is the study of the thermodynamics of QCD in the presence of a nonzero baryonic density, or finite density QCD.

The standard way to include the effects of baryonic matter on QCD vacuum leads to a complex action in the Euclidean formulation and this prevents the use of standard simulation algorithms, based on the idea of importance sampling, defined through a positive definite density of probability, e.g. the exponential of minus the Euclidean action. This problem can be rephrased stating the impossibility of defining a Boltzmann weight for each field configuration: only calculating the partition function can we correctly define the observables and obtain sensible results for quantities of physical interest.

Calculations of partition functions are not infrequent in lattice simulations [1], but their nature of extensive quantities raises the problem of the feasibility of this type of calculation with limited statistics, as forced from finite computing power.

Although a reliable evaluation of the partition function of lattice gauge theories with dynamical fermions at zero baryon density is possible and successful [2], the extension of such a technique for finite density QCD appears out of reach for any reasonable statistics, at least in a range of theory parameters: for some values of the chemical potential μ the phase of the fermionic determinant can be estimated only averaging over $O(e^V)$ configurations [3,4].

In order to have some hints of the finite density QCD behavior the attention has moved to simpler (even if unphysical) models like infinite mass QCD. Despite the problems related with the phase of the Dirac determinant, in the large bare quark masses regime one can hope to obtain reliable results since, for any β in this regime, the interval of chemical potential where the contribution of the phase cannot be numerically evaluated shrinks considerably [5].

The phase diagram of QCD at large quark mass has been studied using numerical [6,7] as well as analytical methods [3]. As a consequence of the numerical simulation results the authors of [6,7] cast doubts on the existence of a deconfining transition at $\mu\neq 0$ and finite temperature, but a clear evidence of this (unexpected) behavior is still lacking. Different approximations (infinite quark mass [6] or truncation of an expansion in a fixed baryon density approach [7]) and the small lattices ($N_t=2$) used could have obscured the transition signal. In order to clarify somewhat the scenario we have decided to investigate if, by simulating true QCD at finite but large masses and $N_t=4$, at $\mu\neq 0$ the theory still has a discontinuous transition.

By monitoring the expectation value of the phase of the Dirac determinant we can distinguish the regions in the parameter space where our evaluation of the partition function of finite density QCD is (in principle) exact from the ones where we miss a possible contribution to $\mathcal{Z}$.

In the next section we will give arguments to explain why the contribution of the phase cannot be measured and will present, in the strong coupling limit, a quantitative check of the grand canonical formulation using results obtained with different techniques. The third section is devoted to the exposition of our approach to simulations of finite density QCD at finite coupling which exploits the main advantage of the microcanonical fermion average (MFA) approach [8], i.e. the free mobility in the (β,μ) plane, and then we present results for fermionic and gluonic observables, discussing the fate of the deconfining phase transition when one increases the baryon density. A coherent picture seems to emerge from our data: a deconfining critical line that, with respect to $\mu=0$, moves towards smaller β with increasing μ.

II. THE PARTITION FUNCTION OF FINITE DENSITY QCD

The finite density QCD partition function can be written as

$$\mathcal{Z}=\int [dU]e^{-\beta S_g(U)}\det\Delta(U,m_q,\mu) \qquad (1)$$

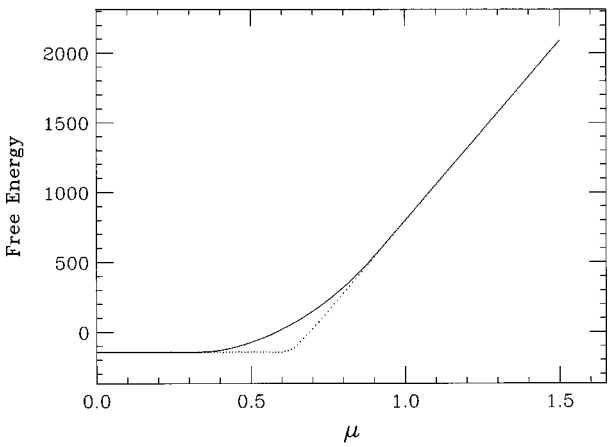

FIG. 1. Free energy at $\beta=0$ and $m_q=0.1$ of true QCD in the MDP approach (dotted line) and of modulus QCD (continuous line).

where, using the staggered formulation, the fermionic matrix Δ takes the standard form [9]

$$\Delta_{i,j}=\frac{1}{2}\sum_{\nu=1,2,3}\eta_\nu(i)[U_\nu(i)\delta_{j,i+\hat{\nu}}-U_\nu^\dagger(i-\hat{\nu})\delta_{j,i-\hat{\nu}}]+\frac{1}{2}[U_4(i)\delta_{j,i+\hat{4}}e^{\mu}-U_4^\dagger(i-\hat{4})\delta_{j,i-\hat{4}}e^{-\mu}]+m_q\delta_{i,j}\,.$$

The contribution of modulus $|\det\Delta|$ of Dirac determinant and its phase ϕ_Δ can be separated as [10]

$$\mathcal{Z}=\mathcal{Z}_\parallel\langle e^{i\phi_\Delta}\rangle_\parallel\,, \tag{2}$$

where

$$\mathcal{Z}_\parallel=\int[dU]e^{-\beta S_g(U)}|\det\Delta(U,m_q,\mu)| \tag{3}$$

is the partition function of the model with the modulus of the determinant (modulus QCD in the following), and

$$\langle e^{i\phi_\Delta}\rangle_\parallel=\frac{\int[dU]e^{-\beta S_G(U)}|\det\Delta|e^{i\phi}}{\int[dU]e^{-\beta S_G(U)}|\det\Delta|}. \tag{4}$$

It is clear from Eq. (2) that, in the thermodynamical limit, the theory defined by means of $\mathcal{Z}_\parallel$ is physically different from the original theory only when the expectation value of the cosine of the phase of fermion determinant is vanishing exponentially with the system volume. In the regions of parameter space where the aforementioned expectation value is not $O(e^{-V})$, modulus QCD is an equivalent formulation of finite density QCD, i.e. indistinguishable in the thermodynamical limit. In the rest of parameter space, modulus QCD clearly overestimates the true QCD partition function.

Let us try to better illustrate this concept looking at Fig. 1. It refers to the infinitely strong coupling limit $\beta=0$ and $V=6^3\times4$. At fixed quark mass m_q the partition function of the system is only dependent on chemical potential μ. If we plot the free energy versus μ we can extract the phase structure from the appearance of a singularity in (some derivative of) the curve.

Two extreme limits are well known. At $\mu=0$ we get the logarithm of the usual fermion determinant averaged over gauge field configurations: an average of a well defined (real and positive) quantity that can be computed. On the other hand in the large μ limit only the last term of the grand canonical partition function (see later) survives: $\det\Delta\rightarrow(1/2)^{3V}e^{3V\mu}$ and the free energy is a straight line with slope $3V$. In this limit the (baryon) number density, defined as

$$N(\mu)=\frac{1}{3V}\frac{\partial}{\partial\mu}\log\mathcal{Z}, \tag{5}$$

is equal to 1, and we can say that we are in a saturation regime, with the Pauli exclusion principle preventing further increase of baryon density. In these two limits modulus QCD is coincident with the true theory and deviations are possible only in the intermediate region.

Starting from $\mu=0$, we can use the data of Fig. 5 in Ref. [11], regarding number density at $m_q=0.1$, in order to reconstruct the free energy of the true theory as seen from the monomer dimer polymer (MDP) approach. This is shown in Fig. 1 as the dotted line. If we superimpose the results of modulus QCD (continuous line) we can easily identify three regions: $\mu<\mu_1\simeq0.3$, which defines the onset in modulus QCD, where the number density is essentially zero; $\mu>\mu_2\simeq1.0$, the saturated region; and $\mu_1<\mu<\mu_2$, the region where modulus QCD grossly overestimates the free energy of true theory. As stated in [12], using the Glasgow prescription [13] for dealing with the complex determinant, we obtain, for the free energy, exactly the same results as in modulus QCD.[1]

In Fig. 2 we report, for the same lattice and quark mass, the difference between the free energy of modulus QCD and the estimation based on data of Ref. [11]. Superimposed to that we plot the expectation value of $\langle e^{i\phi_\Delta}\rangle_\parallel$ at the same value of the parameters. It is evident that the intermediate region is where the phase term is vanishing within statistical errors. If we concentrate on a value of μ inside this region, for example $\mu=0.7$, the distribution of the phase of the fermion determinant of single field configurations is almost flat.

With a statistics of N configurations we can hope to measure accurately the phase term $\langle e^{i\phi_\Delta}\rangle_\parallel$ only down to $O(1/\sqrt{N})$ ($\simeq0.02$ for our runs), far from the $O(e^{-V})$ order needed in principle. Even with a statistics of some thousands of configurations, we can say nothing on free energy of true theory in the range $\mu_1<\mu<\mu_2$, that covers the region where

[1]In light of some recent results [14] serious doubts can be cast on the MDP data in the critical region; however, what is crucial here, actually, is the value of the onset μ for this approach: the more recent analysis moved it down to $\mu=0.6$, still far from onset μ of modulus QCD.

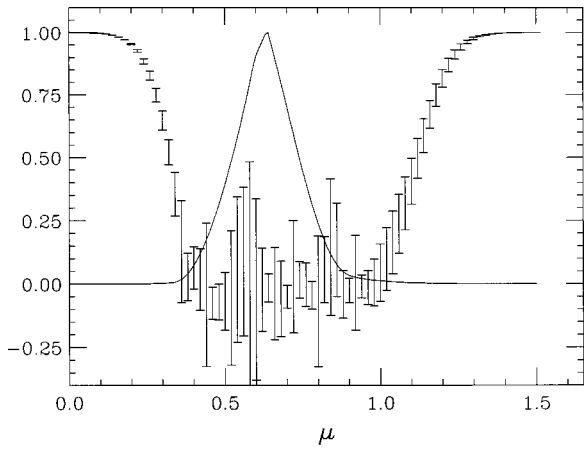

FIG. 2. Normalized difference between the free energy of modulus QCD and the free energy of true QCD in the MDP approach (continuous line) superimposed to the expectation value of the determinant phase at $\beta=0$ and $m_q=0.1$.

the number density varies rapidly. This does not imply necessarily that the phase is relevant in this region: for example it could go to zero as e^{-V_S}, with V_S the spatial volume, being in this case at the same time irrelevant and nonmeasurable.

The situation becomes somewhat better if we move to large quark mass: the range (μ_1,μ_2), where finite statistics effects prevent one from obtaining a sensible evaluation of free energy, becomes narrower and the region between $\mu=0$ and μ_1, where interesting physics can be studied at least at finite temperature, becomes wider. The same scenario holds at finite coupling too, allowing us to investigate a great part of the parameter space. In particular, as we will see in the following, we are interested in the neighborhood of the $\mu=0$ finite temperature critical point, to address the fate of the deconfining transition when baryon density increases.

III. SIMULATION SCHEME AND LARGE QUARK MASS RESULTS

Our simulations are based on the GCPF (grand canonical partition function) formalism [15] with an MFA (microcanonical fermionic average) [8] inspired approach for intermediate coupling analysis.

The basic idea in MFA is the exploitation of the physical equivalence between the canonical and microcanonical formalism via the introduction of an explicit dependence on the pure gauge energy in the computation of the partition function. Indeed Eq. (1) can be written as

$$\mathcal{Z}(\beta,\mu,m)=\int dE n(E) e^{-6V\beta E}\langle S^F_{\rm eff}(\mu,m_q)\rangle_E \qquad (6)$$

where

$$n(E)=\int [dU]\delta(6VE-S_g[U]) \qquad (7)$$

is the density of states at fixed pure gauge energy E, and

$$\langle S^F_{\rm eff}(\mu,m_q)\rangle_E=\frac{\int [dU]\delta(6VE-S_g[U])S^F_{\rm eff}([U],\mu,m_q)}{n(E)} \qquad (8)$$

is the average over gauge field configurations at fixed energy E of a suitable definition of effective fermionic action.

For the calculation of $\langle S^F_{\rm eff}\rangle_E$ we proceed as follows: first, we choose a set of energies selected to cover the range of β we are interested in. Secondly, for all the energies in the set, we generate gauge field configurations using a pseudo-microcanonical code; the generation of gauge fields at fixed energy is not the costly part of the whole procedure, so we can well decorrelate the configurations used for measuring the Dirac operator. Then, a library routine is used in order to obtain the complete set of eigenvalues of the propagator matrix P. At this point we can reconstruct the fugacity expansion coefficients or, without any substantial additional computer cost, use the eigenvalues to explore the possibilities offered by alternative prescriptions for the fermionic effective action, i.e. evaluate the modulus of the determinant and hence $\mathcal{Z}_\parallel$. At the end, we have the fermionic effective action evaluated at discrete energy values: a polynomial interpolation allows the reconstruction at arbitrary values of the energy E, in order to perform the numerical one-dimensional integration in Eq. (6) and obtain the partition function $\mathcal{Z}_\parallel(\beta,\mu,m)$.

In a previous work [12] we have found evidence for numerical instabilities in the evaluation of coefficients, whose origin lies on the ordering of the eigenvalues of P as calculated by a standard diagonalization routine. A random arrangement of the eigenvalues, before the calculation of the coefficients, is necessary in order to control rounding effects. In the present work we have always used this procedure to calculate the GCPF expansion coefficients.

Let us now present our results in the large bare quark mass limit at intermediate coupling finite density QCD. We have performed simulations in a $4^3\times 4$ lattice (10 masses $m_q=1.0\rightarrow 5.0$) in the range of the chemical potential $\mu\in[0.0,4.0]$ and $\beta\in[4.0,6.0]$; we will show the results at $m_q=1.8$ as representative.

If the hadronic and quark-gluon plasma phases have to be separated in the physical parameter space of temperature and chemical potential we have to find evidence for a transition line in the plane of the bare quantities $\beta-\mu$. This line should start from the $\beta_c(\mu=0)$ first order critical point and continue for smaller values of β as μ is increased.

To address this point we have studied the plaquette energy $E(\beta,\mu)$, the Polyakov loop $P(\beta,\mu)$ and the number density as a function of β.

In Figs. 3(a) and 3(b) we report $E(\beta,\mu)$ and $\partial E(\beta,\mu)/\partial\beta$, evaluated at bare quark mass $m_q=1.8$ and at different values of the chemical potential $\mu<\mu_c^S$. In Fig. 3(a) we can clearly see a rapid variation of the observable for all the values of μ; for the $\mu=0$ curve this happens in correspondence with the pseudo-temperature transition of zero density full QCD. The critical gauge coupling moves to smaller β as we increase μ. This phenomenon is also evident

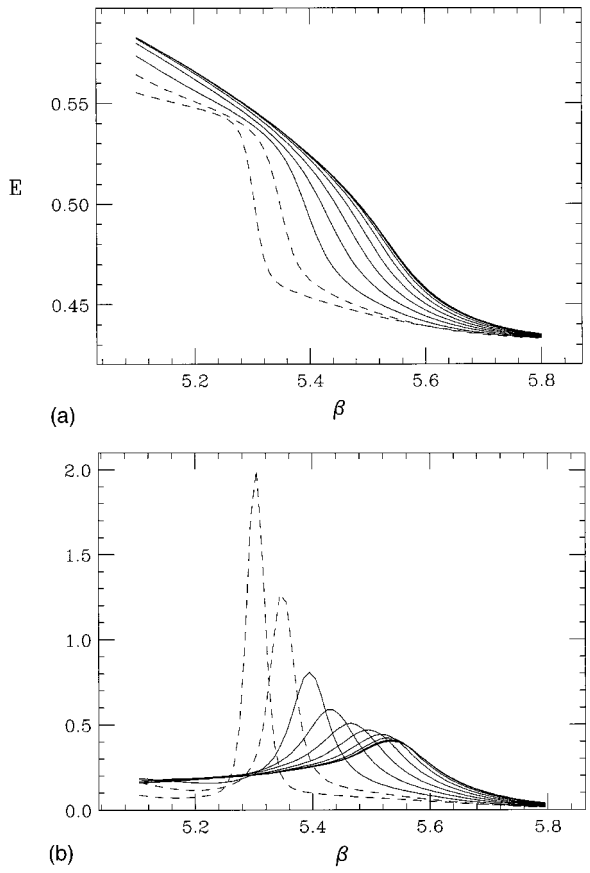

FIG. 3. Plaquette energy $E(\beta,\mu)$ (a) and its derivative $\partial E(\beta,\mu)/\partial\beta$ (b) evaluated in a $4^3\times4$ lattice at $m_q=1.8$ for $\mu=0.0\rightarrow1.5$ (from the right to the left) in steps of 0.1. Dashed lines are for $\mu>\mu_1$.

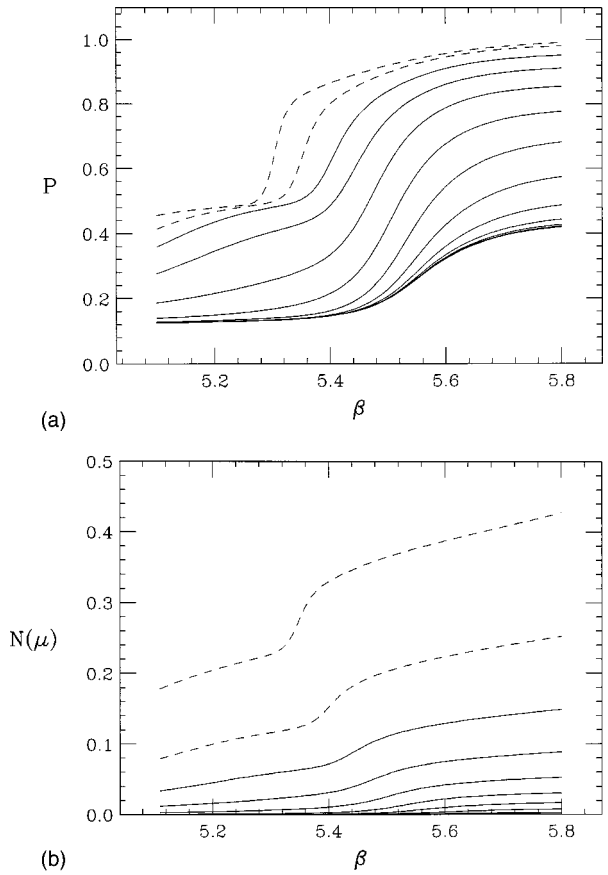

FIG. 4. Polyakov loop $P(\beta,\mu)$ (a) and number density (b) evaluated in a $4^3\times4$ lattice at $m_q=1.8$ for $\mu=0.0\rightarrow1.5$ (from the right to the left) in steps of 0.1. Dashed line are for $\mu>\mu_1$.

as a sharp peak in the figure of the derivative [Fig. 3(b)]. It is tempting to interprete this as an evidence of a temperature induced phase transition extending at nonzero values of μ. Also the behavior of the Polyakov loop points in this direction: as can be seen in Fig. 4(a), $P_\mu(\beta)$ changes rapidly at values of β consistent with the ones obtained from the energy.

We have completed the analysis with the number density results. This observable gives a less clear signal since it is forced to be a constant function of β at $\mu=0$. Nevertheless we can see in Fig. 4(b) that the behavior of this observable is still consistent with previous findings for the gluonic quantities. It is useful to remark that plotting the same quantities at fixed β as a function of μ we would be practically unable to see any signal.

Signals for a developing discontinuity in all these observables rely on data in the region where the contribution of the phase is negligible, but similar behavior is found at larger values of μ, too.

To conclude our analysis we report in Fig. 5 the (β,μ) phase diagram of the theory at $m_q=1.8$ and $V=4^4$.

IV. CONCLUSIONS

In this paper we have studied finite density lattice QCD by means of numerical simulations. As is well known this approach, probably the only one able to tackle the nonperturbative effects leading to quark-gluon plasma transition, suffers severe problems due to the lack of hermiticity of Dirac operator for a single realization of gauge fields.

In the first part of the paper we have shown, as for small quark masses and strong coupling, any numerical algorithm based on the GCPF approach gives results different from what is expected in the region where the contribution of the

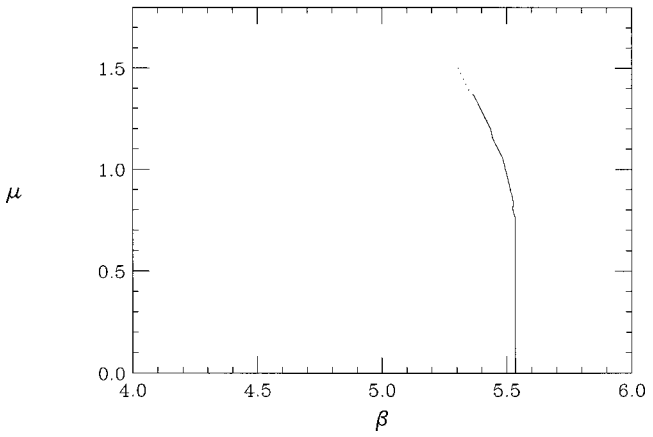

FIG. 5. Phase diagram for the $4^3\times4$ lattice at $m_q=1.8$ in the (β,μ) plane; the dotted line is for $\mu>\mu_1$.

phase cannot be evaluated. To our understanding only a statistics exponentially large with the system volume (and a consequently high accuracy in numerical calculations) can solve this problem.

Moving to the large quark mass region we meet a much better situation and a large part of the parameter space becomes accessible to numerical simulations.

The new result is the evidence of a transition line for true QCD that originates from the critical point of the four flavor $\mu=0$ theory. This has to be regarded as the lattice counterpart of the transition line in the temperature-chemical potential plane that separates the hadronic phase from the quark-gluon plasma phase at large masses.

Concerning this transition, the previous results in literature were not definite, but it has to be stressed that they have been obtained using different approaches and/or approximations. Instead we directly simulate QCD in the large mass limit, and in this limit we obtain a result in qualitative agreement with expectations for a true finite density transition. Due to the differences in methods these results cannot be directly compared; larger lattices could clarify the issue, but the volumes attainable with reasonable computer resources make this program not effective. To extend these results to the small quark mass region is impossible since the contribution of the phase to the partition function becomes practically unmeasurable in the whole parameter space.

At the end we have to conclude that, until now, finite density lattice QCD, far from providing quantitative insights into the behavior of quarks and gluons, can at most give us some qualitative indication.

ACKNOWLEDGMENTS

This work has been partly supported through a CICYT (Spain)–INFN (Italy) collaboration. A.G. was supported by the Istituto Nazionale di Fisica Nucleare at the University of Zaragoza.

[1] G. Bhanot, K. Bitar, and R. Salvador, Phys. Lett. B **188**, 246 (1987); M. Karliner, S. Sharpe, and Y.F. Chang, Nucl. Phys. **B302**, 204 (1988).

[2] V. Azcoiti, I.M. Barbour, R. Burioni, G. Di Carlo, A.F. Grillo, and G. Salina, Phys. Rev. D **51**, 5199 (1995).

[3] R. Aloisio, V. Azcoiti, G. Di Carlo, A. Galante, and A.F. Grillo, Phys. Lett. B **453**, 275 (1999).

[4] I.M. Barbour, Nucl. Phys. **A642**, 251c (1998).

[5] I.M. Barbour, N.E. Behilil, E. Dagotto, F. Karsch, A. Moreo, M. Stone, and H.W. Wyld, Nucl. Phys. B: Field Theory Stat. Syst. **B275**[FS17], 296 (1986).

[6] T. Blum, J.E. Hetrick, and D. Toussaint, Phys. Rev. Lett. **76**, 1019 (1996).

[7] J. Engels, O. Kaczmarek, F. Karsch, and E. Laermann, Nucl. Phys. **B558**, 307 (1999).

[8] V. Azcoiti, G. Di Carlo, and A.F. Grillo, Phys. Rev. Lett. **65**, 2239 (1990); V. Azcoiti, A. Cruz, G. Di Carlo, A.F. Grillo, and A. Vladikas, Phys. Rev. D **43**, 3487 (1991).

[9] J.B. Kogut, H. Matsuoka, M. Stone, H.W. Wyld, S. Shenker, J. Shigemitsu, and D.K. Sinclair, Nucl. Phys. B: Field Theory Stat. Syst. **B225**[FS9], 93 (1983); P. Hasenfratz and F. Karsch, Phys. Lett. **125B**, 308 (1983).

[10] A. Gocksch, Phys. Rev. D **37**, 1014 (1988).

[11] F. Karsch and K.H. Mütter, Nucl. Phys. **B313**, 541 (1989).

[12] R. Aloisio, V. Azcoiti, G. Di Carlo, A. Galante, and A.F. Grillo, Phys. Lett. B **435**, 175 (1998).

[13] I.M. Barbour, S.E. Morrison, E.G. Klepfish, J.B. Kogut, and M.P. Lombardo, Phys. Rev. D **56**, 7063 (1997).

[14] R. Aloisio, V. Azcoiti, G. Di Carlo, A. Galante, and A.F. Grillo, hep-lat/9910015.

[15] P.E. Gibbs, Phys. Lett. B **172**, 53 (1986).