Complex Langevin solution to an effective theory of lattice QCD

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By means of a complex Langevin algorithm, we simulate on the full group space an effective three-dimensional theory of QCD at finite temperature and finite chemical potential. We study the effect of the chemical potential on the first-order character of the deconfinement phase transition.

I. INTRODUCTION

The effects of a finite chemical potential on lattice QCD are still rather poorly known. This is due to the fact that a nonzero chemical potential leads to a complex action if the appearance of a singularity in the naive continuum limit is to be avoided.[1] The main difficulty in working with a complex action is that standard Monte Carlo sampling is no longer applicable. Attempts to use Monte Carlo updating while including the non-positive-definite part of the Boltzmann factor into the operator to be measured[2] are hampered by large fluctuations. The only updating procedure based on the full complex action which seems to offer hope of success at the present time is based on stochastic quantization.[3]

When the action is real, one can prove under very general assumptions that the associated stochastic process converges to the correct equilibrium distribution.[3] The assumptions under which this holds true when the action is complex are not yet known. However, analytic[4] and computer-assisted[5] proofs of proper convergence have been given for specific examples of complex-action theories. In fact, most attempts to simulate complex actions have been successful.[6–10] The counterexamples known so far are actions which are either explicitly unsuitable for simulation (the associated process is nonergodic[10]) or not bounded from below.[11] Therefore, it seems reasonable to hope that even complicated and realistic theories with complex actions can be solved by Langevin quantization, provided the complex extension of the differential equation is formulated properly.

In the present paper, we report the results of a complex Langevin simulation of an effective three-dimensional theory based on QCD in the strong-coupling limit with Wilson quarks at finite temperature and finite chemical potential. For large quark masses, this is expected to be a reasonable model in which to study the structure of the deconfinement phase transition. Moreover, this model is easier to simulate than full QCD with dynamical quarks (which remains the final goal). We have previously solved the analogous U(1) effective model, with encouraging results.[8] This model of QCD is also solvable by mean-field methods,[12] so that we have terms of reference for the complex Langevin results.

Because of the symmetry of this particular model, it is possible to restrict its simulation to a subspace of SU(3) and to its complex extension.[9] We prefer to simulate in the full group space, since the resulting algorithm can be generalized to the full theory. Also, we concentrate on the effect of finite quark mass and chemical potential on the order of the deconfinement phase transition, which has not been studied before.

In Sec. II we present the action to be studied and the mean-field predictions for the phase diagram. Section III contains a short discussion of the complex extension of the Langevin equation, of the numerical algorithm, and of its systematic errors. Our results on the order of the deconfinement transition for zero chemical potential and variable quark mass are presented in Sec. IV, and the results for fixed quark mass and variable finite chemical potential are given in Sec. V. Some conclusions are drawn in Sec. VI.

II. THE MODEL AND ITS MEAN-FIELD ANALYSIS

Starting from SU(3) theory with the standard Wilson action and with Wilson quarks (hopping parameter κ) on a $(d=4)$-dimensional lattice with N_τ temporal sites, one can use the character expansion in the strong-coupling limit[13,14] to derive an effective three-dimensional spin-system-type theory of interacting Polyakov loops. The action of this effective theory reads

$$S=-\beta'\sum_{\langle ij\rangle}(\mathrm{Tr}L_i\mathrm{Tr}L_j^\dagger+\mathrm{Tr}L_i^\dagger\mathrm{Tr}L_j)-\sum_i(h_1\mathrm{Tr}L_i+h_2\mathrm{Tr}L_i^\dagger)\ , \tag{1}$$

where the L_i take values in SU(3) and the indices run over the $d=3$ lattice. The last two terms in the action are the first nonvanishing terms in the hopping-parameter expansion[2] for $N_\tau\leq 3$. Defining $h=2n_f(2\kappa)^{N_\tau}$ (n_f is the number of flavors), we have

$$h_1=h\exp(\mu N_\tau),\quad h_2=h\exp(-\mu N_\tau)\ . \tag{2}$$

where the prescription of Refs. 1 and 15 has been used to incorporate the chemical potential μ (the lattice spacing is set to 1). For $\mu\neq 0$, the action in Eq. (1) becomes com-

plex. However, the corresponding partition function remains positive definite.

The effective coupling β' is related to the inverse coupling $\beta=1/g^2$ of the original four-dimensional theory by the first character coefficient $Z_{1;0}$ (Ref. 14):

$$\beta'=[Z_{1;0}(\beta)]^{N_\tau} \tag{3}$$

with

$$Z_{1;0}=\frac{1}{3Z}\int dL\ \mathrm{Tr}L^\dagger \exp[\beta(\mathrm{Tr}L+\mathrm{Tr}L^\dagger)]\ , \tag{4}$$

where Z is a group integral given by

$$Z=\int dL\ \exp[\beta(\mathrm{Tr}L+\mathrm{Tr}L^\dagger)]\ . \tag{5}$$

The complex action defined in Eq. (1) implies in general $\langle \mathrm{Tr}L_i\rangle\neq\langle \mathrm{Tr}L_i^\dagger\rangle$. Therefore, we define the mean-field free energy as

$$\mathcal{F}_{\mathrm{mf}}=6\beta' M_1 M_2+\mathcal{F}_{\mathrm{ss}}\ , \tag{6}$$

where $M_{1,2}$ denote two real mean fields and $\mathcal{F}_{\mathrm{ss}}$ is a single-site free energy

$$\mathcal{F}_{\mathrm{ss}}=-\ln\left[\int dL\ \exp(a\ \mathrm{Tr}L+b\ \mathrm{Tr}L^\dagger)\right] \tag{7}$$

with the notations

$$a=6\beta' M_1+h_1,\quad b=6\beta' M_2+h_2\ . \tag{8}$$

The function $\mathcal{F}_{\mathrm{mf}}$ has to obey two self-consistency equations:

$$\frac{\partial\mathcal{F}_{\mathrm{mf}}}{\partial M_1}=0,\quad \frac{\partial\mathcal{F}_{\mathrm{mf}}}{\partial M_2}=0\ . \tag{9}$$

The solutions $\bar{M}_1$ and $\bar{M}_2$ of Eqs. 9 are the mean-field expectation values of the Polyakov loops:

$$\langle \mathrm{Tr}L^\dagger\rangle=\bar{M}_1,\quad \langle \mathrm{Tr}L\rangle=\bar{M}_2\ . \tag{10}$$

The function $\mathcal{F}_{\mathrm{ss}}$ can be calculated by expanding the integrand in (7) in a power series of a and b; by numerical summation up to any order we may achieve arbitrary precision.[12] The next step is to solve Eqs. (10) numerically for different values of h and μ.

Let us summarize the result for the case $\mu=0$ (Ref. 14). For $h=0$ (pure gauge theory) there is a first-order phase transition at $\beta'=0.1345$. The transition remains first order for $0\le h<h_c$. $h_c=0.055$ is the critical value at which the transition becomes second order. Above h_c there is no transition.

To investigate $\mu\neq 0$ we have to assume $h<h_c$ since for $h>h_c$ there is no transition for any μ (Ref. 12). If now $h<h_c$ the first-order transition will terminate in a second-order end point at some critical value μ_c which depends on h. We show our results for the values $h=0.01$ and $h=0.04$ in Figs. 1 and 2, respectively. Here and in the numerical simulations we shall use $N_\tau=2$. The first-order metastability region shrinks to a point at $\mu_c=1.19$ for $h=0.01$ and at $\mu_c=0.42$ for $h=0.04$.

The results obtained here from the mean-field analysis will serve as a reference for our numerical simulations.

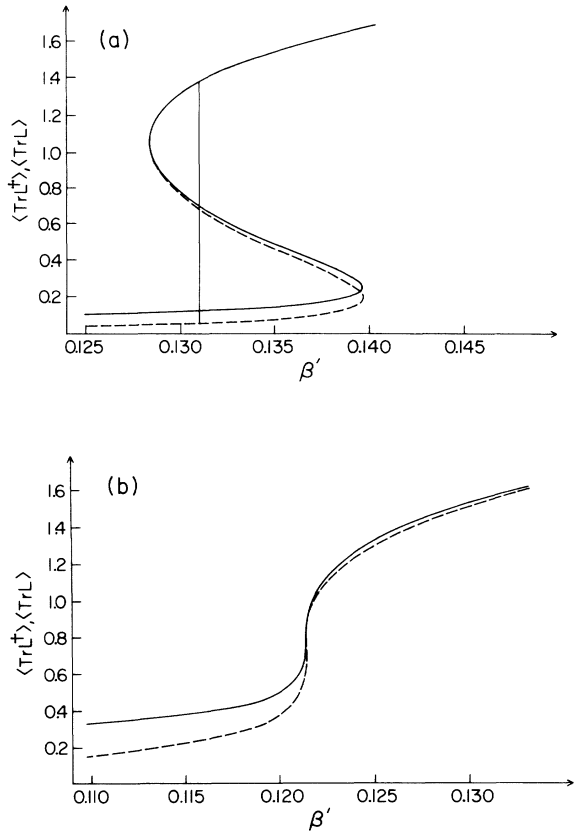

FIG. 1. Mean-field expectation values of the Polyakov loops $\langle \mathrm{Tr}L^\dagger\rangle$ and $\langle \mathrm{Tr}L\rangle$ as a function of β' for $h=0.01$. (a) $\mu=0.5$; (b) $\mu=1.19$. $\langle \mathrm{Tr}L^\dagger\rangle$ and $\langle \mathrm{Tr}L\rangle$ are denoted by the solid and dashed curves, respectively. The solid vertical line in (a) indicates the location of the first-order transition.

III. THE LANGEVIN PROCESS

To simulate the system described in Sec. II, we shall use a Stratonovich-type stochastic differential equation (SDE) in auxiliary time t:

$$dL_i=iL_i(-T^\alpha\nabla_i^\alpha S\,dt+T^\alpha dw_i^\alpha)\ , \tag{11}$$

where w_i^α is a standard Wiener process with covariance

$$\langle w_i^\alpha(t)w_j^\beta(t')\rangle=2\delta_{\alpha\beta}\delta_{ij}\min(t,t')$$

and mean

$$\langle w_i^\alpha(t)\rangle=0\quad(\forall t\ge t_0)\ .$$

α is the SU(3)-color index, i,j run over the sites of a three-dimensional lattice, and T^α are the generators of SU(3) in the fundamental representation ($\mathrm{Tr}T^\alpha T^\beta=\delta_{\alpha\beta}/2$). The operator ∇_i^α is defined as

$$\nabla_i^\alpha=i(L_iT^\alpha)\frac{\partial}{\partial L_i}\ . \tag{12}$$

The SDE (11) is characterized by certain conservation properties.[7,16] To see this, begin by considering S real. Define the real matrices X and Y by $L=X+iY$. One can

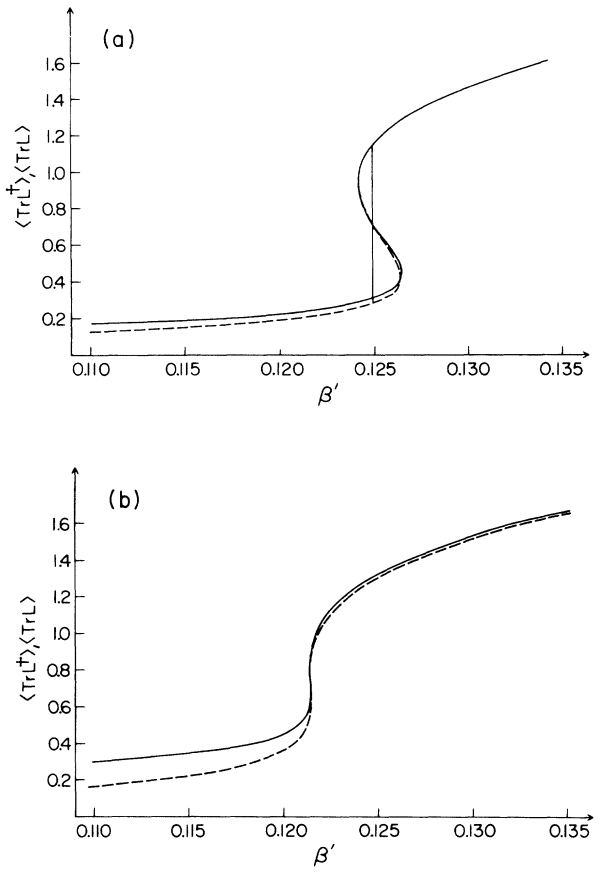

FIG. 2. The same as in Fig. 1 for $h=0.04$ and (a) $\mu=0.01$ and (b) $\mu=0.42$.

then formally split Eq. (11) into real and imaginary parts, yielding a pair of coupled equations for X and Y. These can be shown to preserve the following conditions:[16] (i) $XX^T+YY^T=I$, $XY^T-YX^T=0$; (ii) $\det(X+iY)=1$. In the real-action case, these are just the special unitarity conditions for L.

Consider, however, the extension of the split equations to complex S. Now X, Y are complex matrices, properties (i) and (ii) are still valid but they are no longer equivalent to special unitarity. Therefore, the characteristic conservation properties of the complex Langevin process cannot be derived directly from Eq. (11), but only from the split equations.

Any discretization of these differential equations will violate the above conservation properties.[16] Therefore, the numerical discretization scheme for these processes must include the explicit enforcement of these properties. In the complex-action case, we have seen above that this can only be done at the level of the equations for X and Y. In the present work, we discretize the split equations by means of a two-stage algorithm whose deterministic part is accurate to second order in the auxiliary-time step size ϵ. Conditions (i) and (ii) are implemented as explicit constraints.

The effects of the systematic errors induced by discretization on various lattice observables and on the phase structure have been studied for various theories in the real-action case.[17,18] The additional problem in the complex-action case, as we indicated in the Introduction, is whether an equilibrium action exists at all. If it does, then the analysis of systematic errors should carry over from the real-action case. In particular, the equilibrium action of the stochastic process should be in the same universality class as the simulated field theory. Therefore, we can expect that we should be able to study the phase diagram of our theory even if the step size is large enough to induce a non-negligible systematic error.

However, we must expect that all the couplings in the model, namely, β', h_1, and h_2, will be shifted by the residual systematic error which cannot be eliminated by our second-order scheme.[17] Therefore, the numerical values of the critical parameters observed in our simulation will be subject to systematic uncertainties. To minimize the effect of the bias on our ability to judge the order of the phase transition, we shall compare two independent runs for each value of β, h_1, h_2 which we wish to study: one which starts from a completely ordered configuration and one starting from a completely random configuration. Outside the transition region, the two runs are found to join after a few thousand iterations. We shall therefore consider that a run shows a two-state signal, whenever the hot and cold runs remain widely separated for 10 000 to 14 000 iterations.

All the runs were carried out on a $10\times10\times10$ lattice with periodic boundary conditions. The step size was fixed to $\epsilon=0.01$. This choice should ensure an efficient exploration of phase space while keeping the systematic error tolerably low. In fact, we shall see below that the residual shifts in the critical coupling are indeed small. Of course, as pointed out above, the qualitative nature of the phase diagram is completely unaffected by this systematic error.

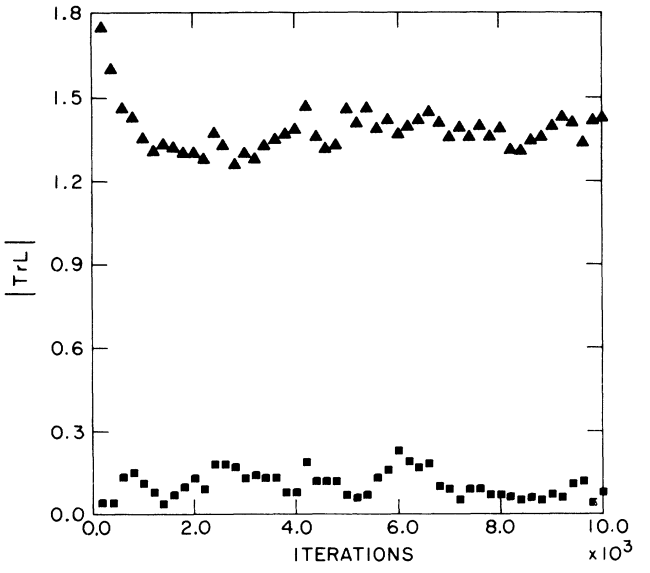

FIG. 3. Time histories for $|\mathrm{Tr}L|$, $h=0$, $\mu=0$, $\beta'=0.136$. Triangles denote the cold run and squares denote the hot run.

IV. RESULTS FOR $\mu=0$

When $\mu=0$, the action given by Eq. (1) is real: $h_1=h_2=h$, $\langle \mathrm{Tr}L_i \rangle = \langle \mathrm{Tr}L_i^\dagger \rangle$. In the limit corresponding to pure gauge theory, $h=0$, the deconfining phase transition is defined by the breakdown of global SU(3) symmetry. Since the ground state of the theory remains symmetric under global Z_3, in Fig. 3 we plot the length of TrL, the lattice average of TrL_i (Ref. 19). In the case $h\neq 0$, the global SU(3) and Z_3 are explicitly broken, so that one could simply plot TrL. However, to be consistent with Fig. 3, the ordinate in Fig. 4 is again the length $|\,\mathrm{Tr}L\,|$. In agreement with the strategy we outlined above, we systematically search for metastability in the time histories of cold and hot runs.

The mean-field analysis has lead us to expect a first-order phase transition for $h=0$ at an effective coupling of $\beta'=0.1345$. The transition is expected to remain first-order for $h<h_c$ and to terminate in a second-order transition point at h_c. There should be a crossover for $h>h_c$. For the value of h_c we have the prediction $h_c=0.055$. The transition β' is expected to decrease as h increases.

Figure 3 shows a clear two-state signal for $h=0$. We find a transition coupling of 0.136 ± 0.004. This agrees, within errors, with the mean-field estimate quoted above as well as with previous numerical determinations.[9,20] This confirms that the Langevin systematic error is indeed small. In Fig. 4 we show how the transition evolves as we increase h (decrease the quark mass from infinity). We observe a rapid weakening of the two-state

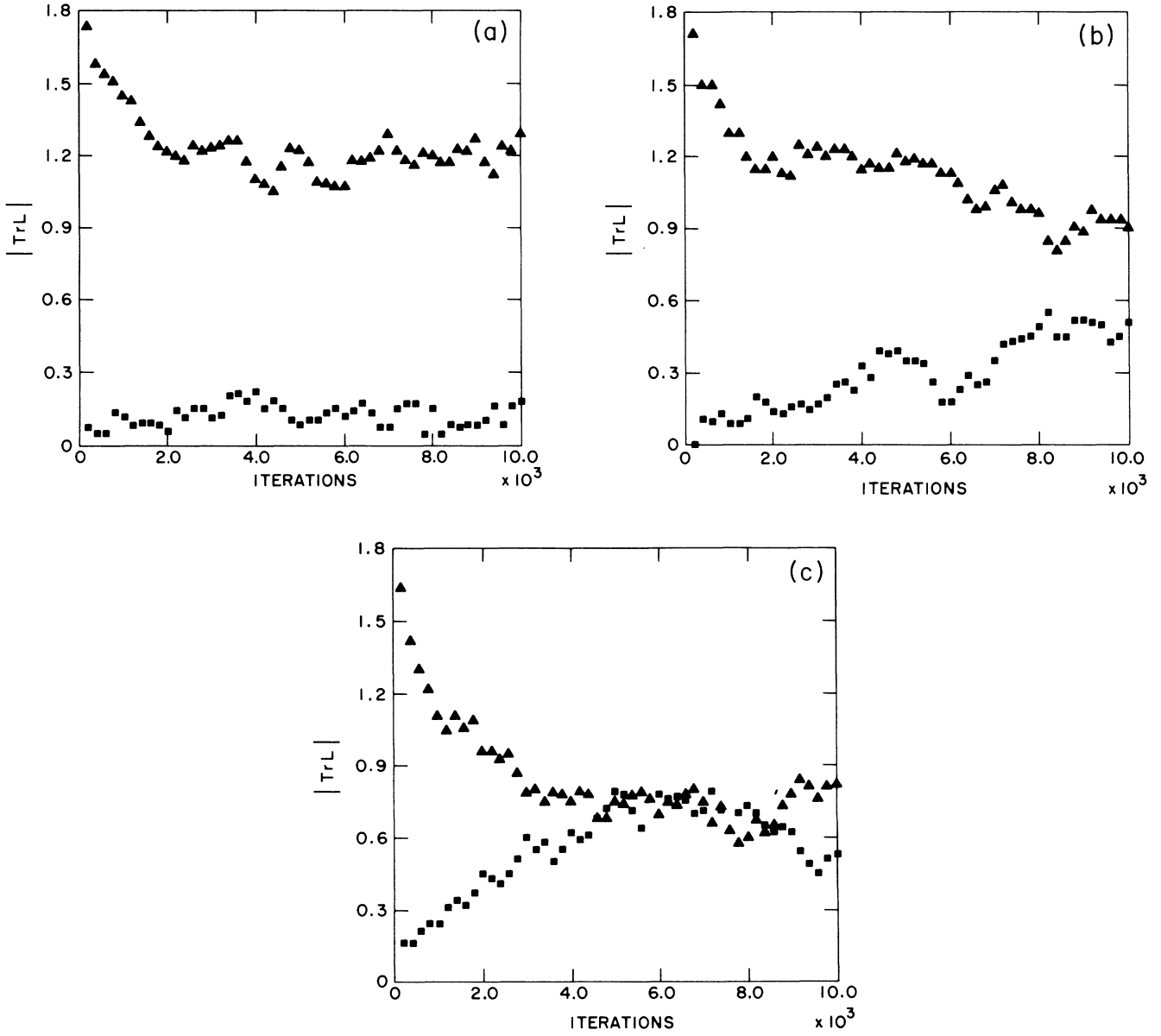

FIG. 4. Same as Fig. 3, but with $\mu=0$ and with various values of h. (a) $h=0.01$, $\beta'=0.134$; (b) $h=0.02$, $\beta'=0.131$; (c) $h=0.04$, $\beta'=0.125$.

signal, which appears to be no longer discernible for $h=0.04$. Since our numerical procedures are not sensitive to the difference between a second-order transition and a rapid crossover, we cannot decide whether the transition terminates abruptly (in a second-order point) or whether it continues as a short second-order line. Note that the critical effective coupling decreases with increasing h, as expected. As the strength of the two-state signal decreases, the range of β' for which metastability is observed narrows by an order of magnitude.

Our present numerical results seem to indicate that the first-order transition vanishes at a lower value of h than that predicted by mean-field theory, and also than the tentative finding reported in Ref. 9. Of course, it is possible that the transition is actually first order for $h=0.04$ and slightly beyond, whereas we cannot resolve a two-state signal as soon as the gap is comparable to the standard deviation of $\mathrm{Tr}L$. However, the transition as observed in Figs. 3 and 4 weakens so fast that the mean-field estimate of h_c is clearly too high. The main difference between our present method of analysis and that of Ref. 9 is that we explicitly search for metastability signals, whereas they draw their conclusions from the dependence of certain observables on the coupling. It is well

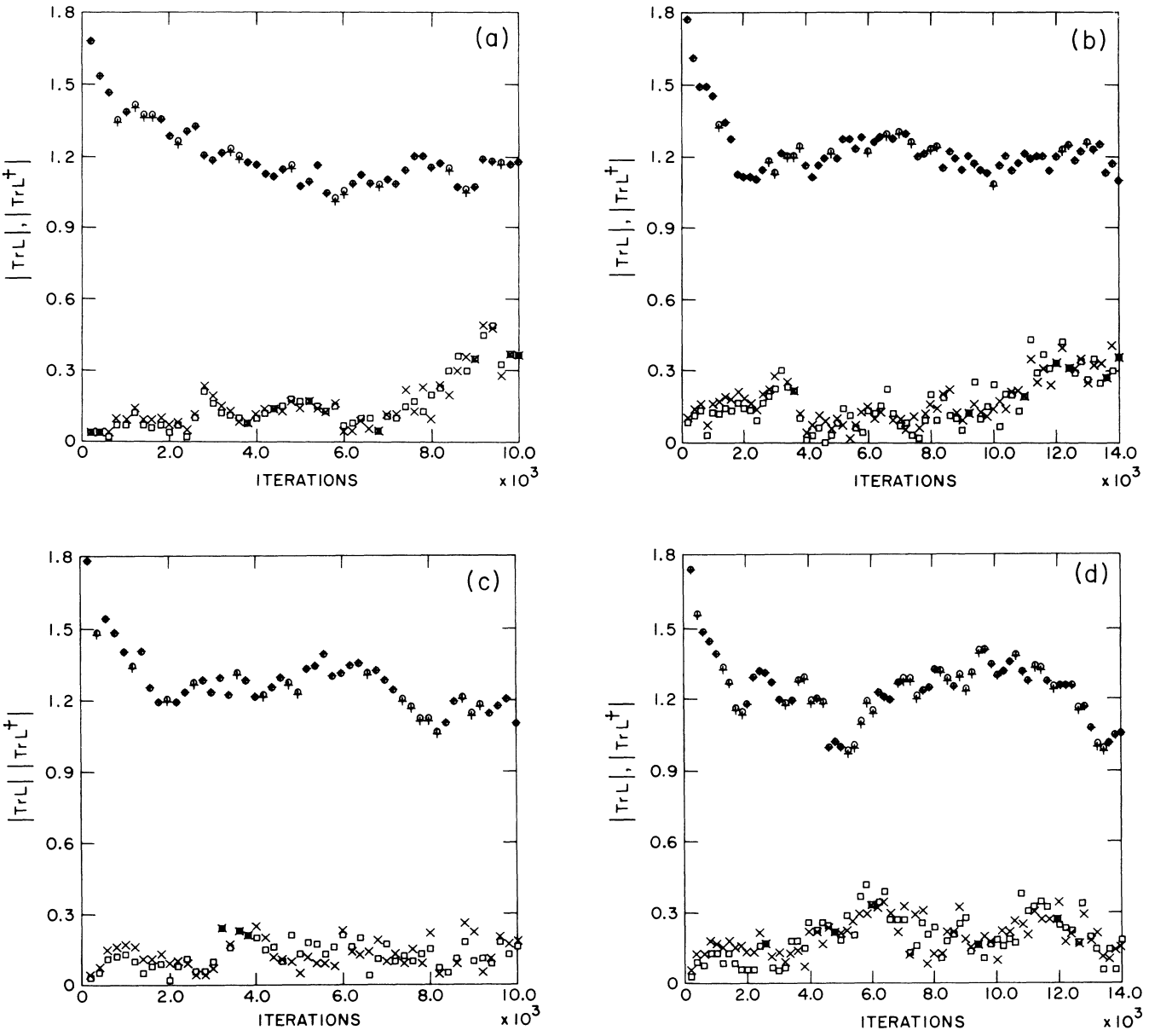

FIG. 5. Time histories for $|\mathrm{Tr}L|$ and $|\mathrm{Tr}L^{\dagger}|$ with $h=0.01$ and various values of μ. Circles and + 's denote the cold runs for $|\mathrm{Tr}L|$ and $|\mathrm{Tr}L^{\dagger}|$, respectively. Squares and $\times$'s denote the corresponding hot runs. (a) $\mu=0.1$, $\beta'=0.133$; (b) $\mu=0.2$, $\beta'=0.1325$; (c) $\mu=0.25$, $\beta'=0.133$; (d) $\mu=0.3$, $\beta'=0.132\,64$; (e) $\mu=0.35$, $\beta'=0.132\,24$; (f) $\mu=0.4$, $\beta'=0.1315$.

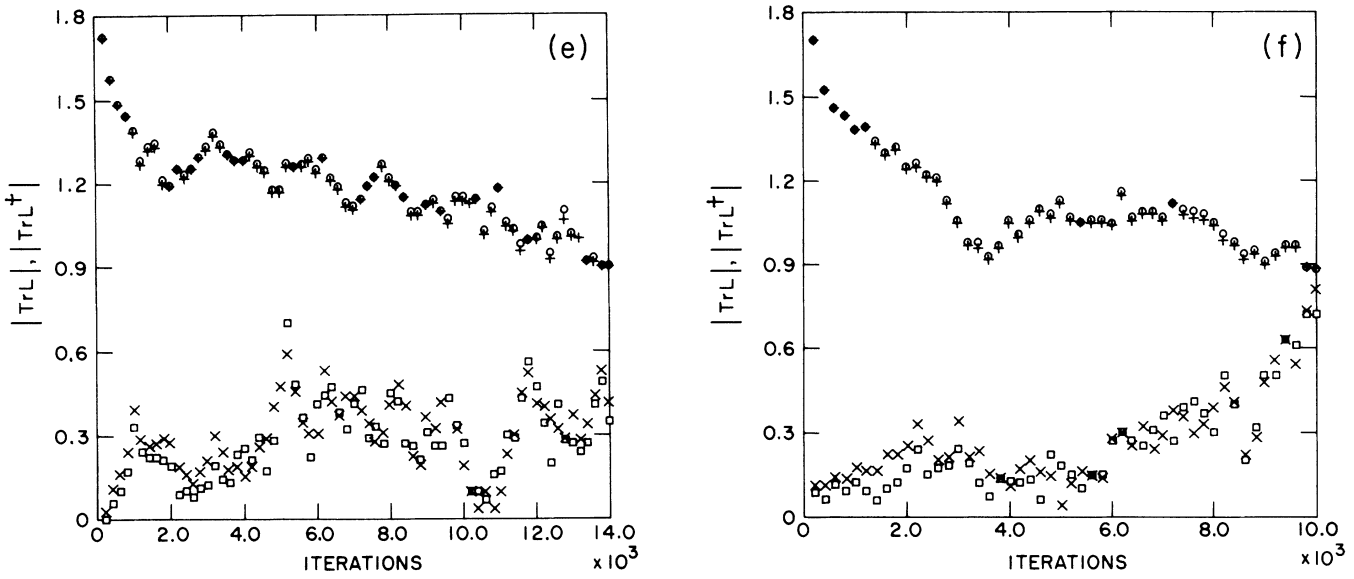

FIG. 5. (*Continued*).

known that these two approaches can lead to quantitatively different conclusions.

V. RESULTS FOR $\mu \neq 0$

When the chemical potential is nonzero, we have $h_1 \neq h_2$; therefore $\langle \mathrm{Tr}L_i \rangle \neq \langle \mathrm{Tr}L_i^\dagger \rangle$ in general. Consider a value of h (of the quark mass) for which the transition was first order for $\mu=0$. By the mean-field analysis of Sec. II we have seen that the effect of increasing μ should be analogous to that of increasing h in the real-action case: the transition should remain first order for $\mu < \mu_c$ and it should terminate in a second-order point at μ_c. There should be a crossover for $\mu > \mu_c$. The transition coupling should decrease with the increase of μ. Our numerical study concentrates on the case $h=0.01$, for which mean-field theory predicts $\mu_c = 1.19$ (see Sec. II).

Another mean-field prediction is that there should be a marked difference between $\mathrm{Tr}L$ and $\mathrm{Tr}L^\dagger$ in the disordered (confined) phase but that this difference should vanish in the ordered (deconfined) phase. To test this we plot the time histories of $|\mathrm{Tr}L^\dagger|$ as well as those of $|\mathrm{Tr}L|$ in Fig. 5.

Figures 5(a)–5(f) suggest that the transition indeed remains first order for $\mu=0.1,0.2,0.25,0.3$ and possibly for $\mu=0.35$. However, it does not appear to be first order for $\mu=0.4$. We have verified that there is clearly no two-state signal for $\mu > 0.4$. The transition coupling is indeed found to decrease with growing μ (within the errors of our procedure); the range of metastability in β' becomes very narrow as μ increases: it is of the order 0.0004 for $h=0.01$, $\mu=0.35$ as compared to 0.004 for $h=0$, $\mu=0$.

We can see that the mean-field prediction concerning the splitting between $\mathrm{Tr}L$ and $\mathrm{Tr}L^\dagger$ as well as the qualitative effect of μ on the phase transition are borne out by the numerical results. On the other hand, the numerical study suggests that the first-order transition disappears at lower μ than mean-field theory predicts.

VI. CONCLUSIONS

We have investigated the phase structure of an effective theory of the deconfinement transition in the presence of a nonzero chemical potential by means of a complex Langevin simulation on the full group space. The qualitative picture which emerges from this numerical study agrees with physical expectations and with the mean-field analysis. For infinitely heavy quarks and zero chemical potential, we recover the well-known result that the deconfinement transition is first order. As the quark mass is decreased (the hopping parameter becomes nonzero), the first-order transition weakens and eventually disappears. If one starts with a value of the hopping parameter for which the transition is first order, the chemical potential has the same effect as a further increase in the hopping parameter: the transition ceases to be first order when μ is large enough. This equivalence is intuitively understandable, since both a decrease in the quark mass and an increase in chemical potential result in more screening. Since it is built into the form of the effective action (1), its appearance in both the mean-field treatment and in the numerical simulation of this theory is in fact not surprising. The present study suggests that the transition ceases to be first order at higher masses and/or lower chemical potential than mean-field theory would predict.

Our successful simulation of the complex extension of a process which diffuses on the SU(3) group manifold is another indication that the SDE approach should work for complex actions which are not manifestly pathological. However, further work on the conditions under which such complex processes converge is clearly needed. In particular, a careful verification of the proper convergence for certain known limits would be important.

As we pointed out earlier, the algorithm used in this work is readily generalizable to the full QCD problem with dynamical quarks. It is known that the light fermions can be simulated by means of additional bilinear

noise terms.[17] This amounts to an additional "heating" of the system, while the main mathematical structure of the problem remains unchanged.

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