Monte Carlo Calculation of Lattice QCD with Exact Treatment of Dynamical Quark Loops

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(Received 3 February 1987)

We study the effects of Wilson fermions in SU(3) lattice gauge theory by an algorithm considering the fermion determinant exactly. We use lattices of size $4^3\times 2$ and 4^4. A comparison is made with the outcomes of fast approximate algorithms of the bush-factorized type. Our results point to the occurrence of a phase transition near $\beta=5.3$ and $\kappa=0.14$. We discuss the relation of this phase transition to that observed recently with the Kogut-Susskind–type fermionic action.

PACS numbers: 12.38.Gc, 11.15.Ha

At present Monte Carlo simulations are the only available mathematical tool for a quantitative study of nonperturbative phenomena in QCD. The investigations, however, have to cope with the enormous computational expenditure associated with the appearance of the fermion determinant in the partition function. This highly nonlocal object may be handled on different levels of sophistication which are as follows: (a) It is ignored ("quenched approximation"), (b) it is taken into account approximately, and (c) it is considered exactly. Exact-algorithm calculations have up to now been done only for Kogut-Susskind fermions.[1-4]

We present in this paper the first results from an exact-algorithm treatment of QCD with Wilson fermions. Present-day computer resources limit this kind of investigation to lattices of rather modest size such as $4^3\times 2$ and 4^4, which have been chosen here.

One of the main purposes for working out exact algorithms which are free from any bias is to obtain data which can serve as a standard for the check of approximate algorithms for systematic errors. Consequently, as a part of our work we compare them to the results of recently proposed approximate methods of the so-called "bush-factorization" type.[5,6]

A second domain of interest is the study of the region toward small quark masses, which is not easily accessible within an approximate algorithm. In particular we want to know if in the approach to the region of light quarks a phase transition would occur as has been observed[4] for the case of Kogut-Susskind fermions.

The system is described by its partition function,

$$Z=\int \mathcal{D}U \exp[-S_{\rm YM}(U)]\{\det W(U)\}^f,$$

for f flavors ($f=3$ in the simulation here), where for the Yang-Mills action $S_{\rm YM}$ we choose Wilson's plaquette action, $S_{\rm YM}=-(\beta/3)\sum \mathrm{Re}(\mathrm{Tr}U_\Box)$, while the fermion matrix is $W=I-\kappa Q$, with hopping matrix

$$Q_{m,n}=\sum[(1-\gamma^\mu)U_{m,\mu}\delta_{n,m+\mu}+(1+\gamma^\mu)U^\dagger_{n,\mu}\delta_{m,n+\mu}].$$

The Monte Carlo treatment consists of building up a Markov chain: An old field configuration $\{U\}$ is replaced by a new one $\{U+\Delta U\}$ according to the probability measure $\exp(-\Delta S_{\rm YM})\rho$, where

$$\rho=\{\det W(U+\Delta U)/\det W(U)\}^f$$
$$=\{\det(I+W^{-1}\Delta W)\}^f.$$

As updating strategy we have chosen the "hypercube updating."[2] We update every link of a fixed four-dimensional unit hypercube five times with ten Metropolis hits before proceeding to the next hypercube. For each hypercube we first calculate the required elements of W^{-1} by the conjugate gradient/residual technique with preconditioning (using the matrix $I+\kappa Q$ for the approximate inverse). The iterations begin from a starting vector obtained approximately with the help of the hopping parameter expansion (HOPE). We then renew the elements of W^{-1} corresponding to the hypercube using Woodbury's formula.[7-9] We discuss the details of the algorithm and the error propagation analysis elsewhere.[10]

The two methods of approximation which we compare here with the exact method are the "bush-factorized Metropolis algorithm"[5] and the "bush-factorized noisy algorithm."[6] Both of them are based on the pseudofermion technique[11,12] in which we express ρ by $\langle\langle\exp(-\Delta S_{\rm PF})\rangle\rangle^{-f/2}$.[13] Here $\Delta S_{\rm PF}$ is the change of the pseudofermionic action $S_{\rm PF}$ under the updating and $\langle\langle\cdots\rangle\rangle$ stands for the average with respect to the distribution $\exp(-S_{\rm PF})$. Upon updating of a set ("bush") of nontouching links the total change of the action is given by $\Delta S_{\rm PF}=\sum_j \Delta_j S_{\rm PF}$ where Δ_j denotes the individual change attributed to the single link j. The approximation consists of replacing ρ by a factorized one, i.e.,

$$\langle\langle \textstyle\prod_j \exp(-\Delta_j S_{\rm PF})\rangle\rangle \rightarrow \prod_j \langle\langle \exp(-\Delta_j S_{\rm PF})\rangle\rangle.$$

In updating a bush, one prepares new gauge fields according to $S_{\rm YM}$ and then accepts the change with the probability in the framework of either the Metropolis algorithm or the "noisy" algorithm of Kennedy and Kuti.[14] The second method is much faster, although it has an "artificially" increased rejection rate, which leads to more correlation between sweeps. Since the approximation error can be controlled and since the step size is not restricted, this method is very successful; it allowed us, e.g., to see hadronization effects on a $8^3\times 4$ lattice.[6]

In the following we want to give our results for several measurable quantities: plaquette average $E_{\rm plq}=\frac{1}{3}\langle {\rm Re}({\rm Tr}U_\Box)\rangle$, Polyakov line $L=\frac{1}{3}\langle {\rm Re}({\rm Tr}U_t)\rangle$, gluon energy $E_G=3\beta\{E_{\rm plq}({\rm timelike})-E_{\rm plq}({\rm spacelike})\}$, and fermion condensate $\langle\bar\psi\psi\rangle=\langle {\rm Tr}(W^{-1})\rangle/{\rm Tr}(I)$.

The results of our investigation on the $4^3\times 2$ lattice for a selected set of parameter values around $\beta=4.0$ and $\kappa=0.12$ are presented in Table I. In addition to the exact- and the approximate- (bush-factorized Metropolis) algorithm data we have included the results from the quenched approximation and from the lowest- (second-) order HOPE. We find good agreement between the exact and the approximate methods. Another observation is that for large and intermediate quark masses the dominant effects are already given by HOPE. This is, however, specific for lattices with time length $N_t=2$, which have a second-order term in the HOPE.

Our results for the 4^4 lattice have been obtained at $\beta=5.3$ and $\kappa=0.13$, 0.14, and 0.15. In Fig. 1(a) we

TABLE I. Plaquette average, Polyakov line, and gluon energy density obtained by different methods on a $4^3\times 2$ lattice with antiperiodic boundary conditions. The lattices are heated first with pure Yang-Mills action for several thousand sweeps; after turning on of the fermions and very fast equilibration, up to 200 sweeps are done for measuring. The given errors are statistical ones and for the approximate method (bush-factorized Metropolis algorithm) include the (estimated) systematic errors, too.

β	κ	Method	$E_{\rm plq}$	$E_G/(2T)^4$	L
3.8	0.12	Exact	0.297(12)	0.44(3)	0.315(13)
		Approx.			
		HOPE	0.2884(4)	0.293(6)	0.293(2)
		Quench.	0.272(2)	0.00	≈ 0
4.0	0.10	Exact	0.303(3)	0.22(2)	0.228(9)
		Approx.			
		HOPE	0.303(4)	0.174(8)	0.210(2)
		Quench.	0.290(2)	0.00	≈ 0
4.0	0.12	Exact	0.323(6)	0.54(3)	0.374(6)
		Approx.	0.320(3)	0.33(3)	0.40(3)
		HOPE	0.320(5)	0.438(8)	0.338(2)
		Quench.	0.290(2)	0.00	≈ 0
4.0	0.14	Exact	0.349(8)	0.86(3)	0.478(4)
		Approx.			
		HOPE	0.342(6)	0.707(10)	0.444(2)
		Quench.	0.290(2)	0.00	≈ 0
4.2	0.12	Exact	0.353(7)	0.71(3)	0.418(5)
		Approx.	0.355(4)	0.63(6)	0.405(30)
		HOPE	0.343(1)	0.61(1)	0.394(2)
		Quench.	0.309(2)	0.00	≈ 0
4.4	0.12	Exact	0.392(8)	0.97(3)	0.485(4)
		Approx.	0.395(5)	0.92(8)	0.50(4)
		HOPE	0.377(1)	0.82(1)	0.456(2)
		Quench.	0.328(2)	0.00	≈ 0
4.6	0.12	Exact	0.429(9)	1.11(2)	0.533(3)
		Approx.			
		HOPE	0.415(1)	1.03(1)	0.515(2)
		Quench.	0.352(2)	0.00	≈ 0

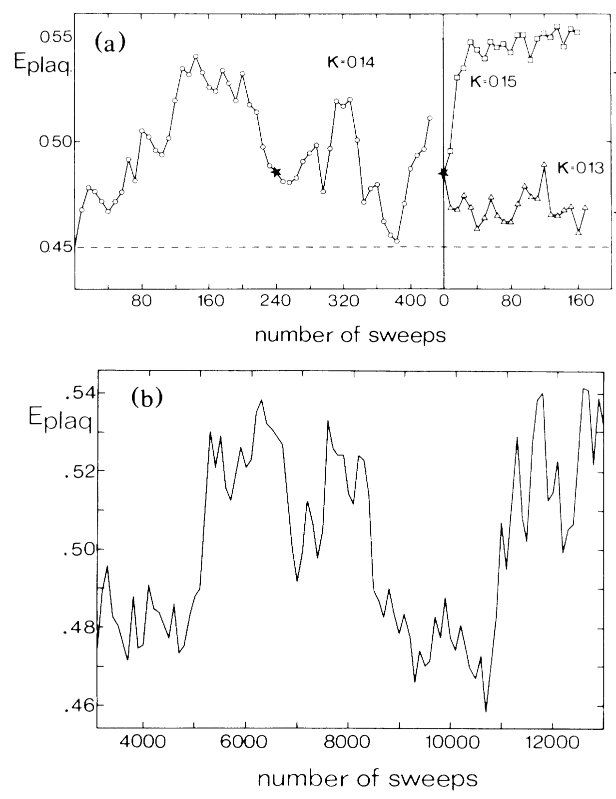

FIG. 1. Plaquette averages of Monte Carlo runs on a 4^4 lattice at $\beta=5.3$ vs sweep number, from (a) the exact method and (b) the bush-factorized noisy algorithm. In (a) the simulation at $\kappa=0.14$ starts with a Yang-Mills equilibrium configuration and at $\kappa=0.13$ and 0.15 with the 240th configuration of the $\kappa=0.14$ sample. The arrows in (a) show the plaquette averages obtained by the bush-factorized noisy algorithm at $\kappa=0.13$ and 0.15, where the value for $\kappa=0.15$ corresponds to the time-space plaquette on a $8^3\times 4$ lattice and therefore represents a lower bound for the plaquette on a 4^4 lattice.

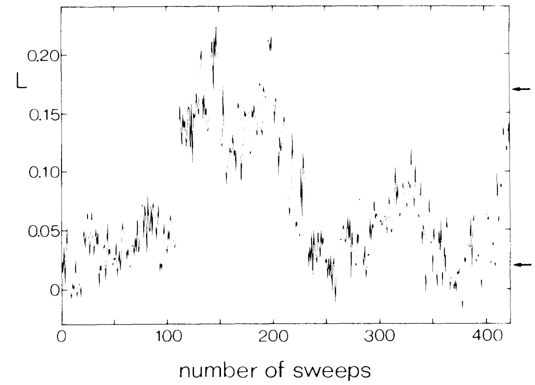

FIG. 2. Polyakov line L on a 4^4 lattice at $\beta=5.3$ and $\kappa=0.14$ vs sweep number (obtained by the exact algorithm) (L means average over Polyakov lines in all space-time directions). The arrows show the two corresponding values of L obtained by the bush-factorized noisy algorithm.

have plotted the exact-algorithm data for the plaquette average as a function of sweeps at $\kappa=0.14$, where every datum point stands for an average over eight sweeps. We see an indication that the system jumps between two different levels during sweeping. We also took data at $\kappa=0.13$ and 0.15, starting from the same configuration (the 240th of our $\kappa=0.14$ sample). They seem to converge to values near the lower and the upper levels at $\kappa=0.14$, respectively. This is further support for the conjecture of two-phase coexistence. For further check, we give in Fig. 1(b) the corresponding results for $\beta=5.3$ and $\kappa=0.14$ from a bush-factorized noisy calculation. We see quite a similar behavior which, however, needs many more sweeps to show up. The agreement between the data obtained by the exact and bush-factorized methods on the 4^4 lattice is good.

In Fig. 2 we present the values for the Polyakov line and in Fig. 3 the results for the fermion condensate. Again the individual behavior of these quantities as well as their strong correlation among each other and with the plaquette average clearly indicate the presence of a two-phase structure. Although $\langle\bar{\psi}\psi\rangle$ calculated with the Wilson-fermion action is not an order parameter for the chiral-symmetry breaking, it is related to the behavior of the fermionic determinant through

$$d[\ln(\det W)]/d\kappa=(1-\langle\bar{\psi}\psi\rangle)\mathrm{Tr}(I).$$

Hence Fig. 3 suggests different eigenvalue distributions of W within the two phases.

Recently another group[4] has claimed to see "clear evidence of chiral-symmetry transition" on a 4^4 lattice from an exact-algorithm treatment but with Kogut-Susskind fermions. They have found a two-phase structure in the behavior of the Polyakov line and of the fermionic condensate at $\beta=4.9$ and $m_a=0.025$, but not any more at $m_a=0.05$, where m_a is the quark mass in lattice units. Do both investigations indicate the same phase transi-

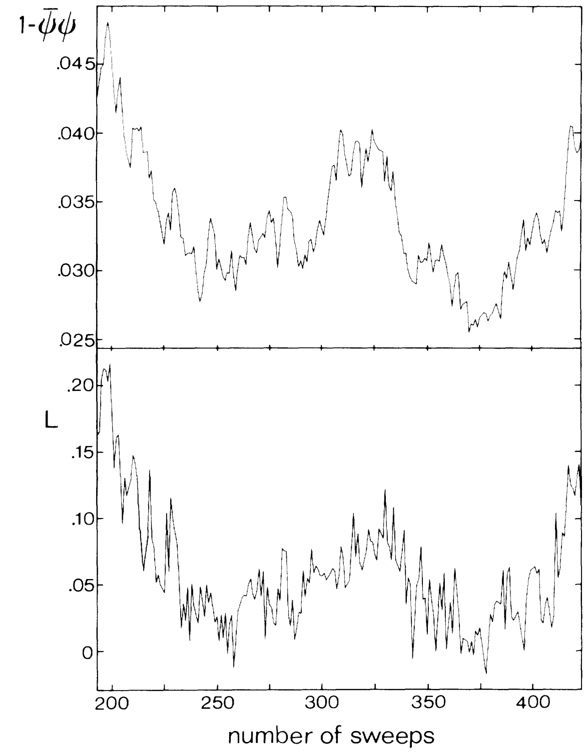

FIG. 3. $1-\langle\bar{\psi}\psi\rangle$ and L on a 4^4 lattice at $\beta=5.3$ and $\kappa=0.14$ (results are obtained by the exact algorithm).

tion? Notice that in our case the chiral symmetry is explicitly broken by Wilson's fermion action. Furthermore our quark mass is very probably much higher. But the behavior of the Polyakov line is very similar to that in Ref. 4. We therefore cannot exclude the possibility that we observe the same transition as in Ref. 4 which then appears at much higher Wilson fermion mass than Kogut-Susskind fermion mass. In this case, however, the dynamical origin of the transition is not clear to us and needs further investigation.

Finally let us mention the performance of our exact algorithm. One sweep on a 4^4 lattice takes on a VP200 roughly 10, 13, and 18 min for $\kappa=0.13$, 0.14, and 0.15, respectively, and half of these on a VP400. The exact algorithm has been run on the VP200 and VP400 at Fujitsu Ltd. and the Cray 1M at Zentrum für Informationtechnik Berlin ZIB, while the approximate algorithms have been run on the Cray 1M at ZIB and the Cray XMP's at Cray Research.

We would like to thank Fujitsu Ltd. (Tokyo) and likewise Cray Research (Minneapolis) for generously offering computational resources on their vector machines. We acknowledge central processing unit time on the vector processor at ZIB. We would like to express appreciation to G. Feuer for his help at the early stage of this work. Two of us (M.H. and A.N.) are much indebted to Y. Tago for his continuous interest and encouragement. One of us (A.N.) thanks K. Sai for his encouragement and the Deutsche Forschungsgemeinschaft for financial support which made his visit to Tokyo possible. He also appreciates helpful discussions with T. Matsui.

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