# Effects of dynamical quark loops on Monte Carlo simulation in lattice gauge theory

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We have run computer simulations in SU(2) lattice gauge theory including dynamical quark loops. We report the experimental results of the plaquette energy, the plaquette-plaquette correlations, $\langle\bar{\psi}\psi\rangle$, the value of the Polyakov line, and $\pi$, $\rho$, and $\omega$ masses and discuss the effects of dynamical quark loops on these quantities. We also present our experimental procedure of the simulations in detail.

## I. INTRODUCTION

The incorporation of fermionic degrees of freedom in Monte Carlo (MC) simulations of lattice gauge theories would allow us to reach a new stage of hadron physics. We could calculate, in principle, all the hadronic properties and could see how the QCD vacuum is constructed at low energies.

Unfortunately, we now stand far from such a state. The main difficulty consists in the very long computational time of quark propagators and, especially, of quark vacuum polarization diagrams. Therefore, the first trials to calculate fermion propagators under SU($N$) gauge fields have been done without quark loops (quenched approximation).[1] The results were quite encouraging: reasonable values of hadron masses, decay constants, and baryon magnetic moments have been obtained. After these successful papers, a flood of efforts have been devoted to the improvement of the results along this line towards larger lattices.[2]

However, the real world includes quark loops. We expect that the mass splitting between the flavor-singlet and -nonsinglet mesons can be explained with quark loops. Chiral symmetry breaking[3] should be confirmed with the inclusion of quark loops.

The hopping-parameter expansion had been the only way to include fermion loops numerically.[4] It is a very good and effective approximation for heavy quarks, i.e., small values of the hopping parameter, and for a small lattice. Fake quark loops due to finite-size effects are easily eliminated in this approximation. However, there is a convergence problem for light quarks, and the computational task is very heavy for a large lattice.

Although the above approaches may be highroads, it is worthwhile, we believe, to explore the MC simulation of gauge theories without these approximations. Towards the real QCD simulations, we should develop efficient algorithms not only for quark propagators but also for quark loops.

The first numerical results along this line were obtained by two of us[5] for SU(2) gauge group and the Wilson action[6] and by Hamber, Marinari, Parisi, and Rebbi[7] for SU(3) and the Kogut-Susskind action.[8] Here we shall continue the study of the previous paper and report more detailed results. In Sec. II, the basic formulas are recalled and several relations are derived which will be useful later. In Sec. III, we describe the experimental procedure and the results. Section IV is devoted to a summary of the problems found in this experiment and to discussing possible approaches to them.

## II. FERMIONS IN THE MC SIMULATION

### A. General formulation

The Euclidean lattice action has the form

$$S=S_G(U)+S_F(U,\bar{\psi},\psi)\ , \tag{1}$$

where the first term represents the kinetic term of gauge variables $U$ with bare coupling $g$. In this paper we employ the Wilson action[6] both for gauge and fermion parts. The fermion action is bilinear in the fermion fields,

$$S_F=\bar{\psi}\Delta\psi=\bar{\psi}(c-kM)\psi\ . \tag{2}$$

The matrix $\Delta$ has the form

$$\Delta=c\delta_{n,m}-k\sum_{\mu=1}^{4}[(r-\gamma_\mu)U_{n,\mu}\delta_{n+\hat{\mu},m} +(r+\gamma_\mu)U^{\dagger}_{m,\mu}\delta_{n,m+\hat{\mu}}]\ , \tag{3}$$

where $n$ and $m$ are site indices and we suppress color and flavor indices. The hopping parameter $k$ is related to the bare mass $m$, Wilson term $r$, and lattice spacing $a$ as

$$k=\frac{c}{8r+2ma}\ . \tag{4}$$

The fermion variables are related to the continuum fermion fields $\psi(x)$ as

$$\psi_n\sim\left[\frac{a^3}{2k}\right]^{1/2}\psi(x)\ .$$

In this paper we set both $r$ and $c$ to be 1. We use self-adjoint Euclidean Dirac matrices:

 

$$\{\gamma^\mu,\gamma^\nu\}=2\delta_{\mu\nu},\quad \gamma^{\mu\dagger}=\gamma^\mu,\quad \mu=1,2,3,4$$
$$\gamma^5=\gamma^1\gamma^2\gamma^3\gamma^4 .$$

The matrix $\Delta$ has the following property:

$$\gamma^5\Delta\gamma^5=\Delta^\dagger . \tag{5}$$

Because of this symmetry, the eigenvalues of $\Delta$ (and $\Delta^{-1}$) appear in complex-conjugate pairs.

For numerical simulations, it is convenient to integrate the partition function over fermion fields using the Matthews-Salam formula

$$Z=\int \mathscr{D}U\,\mathscr{D}\bar{\psi}\,\mathscr{D}\psi\, e^{-S_G-\bar{\psi}\Delta\psi}$$
$$=\int \mathscr{D}U\, e^{-S_G}\det(-\Delta)=\int \mathscr{D}U\, e^{-S_G-S_{\rm EF}} . \tag{6}$$

To our knowledge, there is no proof to show the positivity of $\det\Delta$ above $k=\frac{1}{8}$. We assume, therefore, its positivity. Then we can write

$$\det\Delta=(\det\Omega)^{1/2} , \tag{7}$$

where

$$\Omega=\Delta^\dagger\Delta .$$

For small change of the gauge fields,

$$\delta S_{\rm EF}=-\tfrac{1}{2}{\rm Tr}(\Omega^{-1}\delta\Omega) . \tag{8}$$

We may write meson fields in the form

$$\bar{\psi}(x)\Gamma\psi(x) ,$$

where $\Gamma$ is a matrix with dirac and flavor indices. Then, meson propagators are given by

$$G(x,y)=\langle\,\mathscr{G}(x,y)\rangle , \tag{9}$$

where

$$\mathscr{G}(x,y)=\mathscr{G}_{dc}-\mathscr{G}_c$$
$$={\rm Tr}[\Gamma\Delta^{-1}(x,x)]{\rm Tr}[\tilde{\Gamma}\Delta^{-1}(y,y)]$$
$$-{\rm Tr}[\Gamma\Delta^{-1}(x,y)\tilde{\Gamma}\Delta^{-1}(y,x)] \tag{10}$$

with $\tilde{\Gamma}=\gamma^4\Gamma^\dagger\gamma^4$ and

$$\langle\,\mathscr{G}\,\rangle=\frac{\int \mathscr{D}U\,\mathscr{G}\,e^{-S_G-S_{\rm EF}}}{\int \mathscr{D}U\,e^{-S_G-S_{\rm EF}}} .$$

Figure 1 is a diagrammatic representation of Eq. (10). Except for flavor-singlet mesons, the first term of Eq. (10) vanishes. The time-slice propagators are defined as

$$G(\tau)=\sum_{\substack{x,y\\ x_4-y_4=\tau}} G(x,y) . \tag{11}$$

These propagators, for periodic boundary conditions, show the following behavior at large $\tau$:

$$G(\tau)\sim\cosh Ma\left[\tau-\frac{T}{2}\right] . \tag{12}$$

In this expression, $M$ is the lightest hadron mass with the same quantum numbers as $\bar{\psi}\Gamma\psi$, and $T$ is periodicity in the time direction.

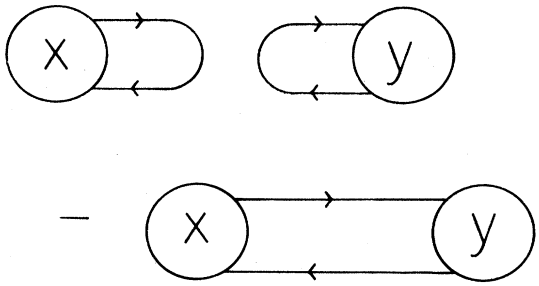


FIG. 1. Diagrammatic representation of the fermion contribution to the meson propagator [Eq. (10)]. The first graph represents the quark-loop contribution to the meson propagator, which is different from zero only for flavor-singlet mesons.

With the help of the Matthews-Salam formula, we can easily get the formula

$$k\frac{d}{dk}\ln\det\Delta={\rm tr}(1)-{\rm tr}(\Delta^{-1}) . \tag{13}$$

After integration over the gauge fields we have

$$k\frac{d}{dk}\langle S_{\rm EF}\rangle=n_f N^4[\langle\bar{\psi}(x)\psi(x)\rangle-4n_c] , \tag{14}$$

where $n_f$ and $n_c$ are the number of flavors and colors, respectively, and $N^4$ is the number of lattice sites. We will use formula (14) later to estimate the magnitude of the effective fermion action, $S_{\rm EF}$.

### B. Pseudofermion method and quark propagators

The pseudofermion MC method was introduced by Fucito, Marinari, Parisi, and Rebbi[9] to calculate $\Delta^{-1}$. The quark propagators, $\Delta^{-1}$, may be expressed in a bosonic integration form,

$$\Delta^{-1}{}_{ij}=\langle\chi_j^*\phi_i\rangle_{\rm PF} , \tag{15}$$

where

$$\langle\theta\rangle_{\rm PF}=\frac{\int \mathscr{D}\phi^*\mathscr{D}\phi\,\theta e^{-S\phi}}{\int \mathscr{D}\phi^*\mathscr{D}\phi\, e^{-S\phi}} \tag{16}$$

and

$$\chi=\Delta\phi . \tag{17}$$

The bosonic fields, $\phi$, have the same quantum numbers as $\psi$. The "action" $S_\phi$, being positive definite, is given by

$$S_\phi=\chi^\dagger\chi . \tag{18}$$

Fucito *et al.* have proposed to evaluate this integral by the MC method.

In terms of the pseudofermion fields, the variation (8) may be expressed in the form

$$\delta S_{\rm EF}=-\langle\chi^\dagger(\delta\Delta\phi)\rangle_{\rm PF} . \tag{19}$$

Since the gauge and the pseudofermion MC sweeps of a lattice are performed in turn, we do not know the new gauge configuration $\{U_{\text{new}}\}$ and, therefore, the variation $\delta\Delta$ in Eq. (19) during the updating of the pseudofermion variables. We rewrite $\delta\Delta$ in the following form:

$$\delta\Delta=-k\sum_{\mu=1}^{4}[(1-\gamma_\mu)(DU)_{n,\mu}\delta_{n+\hat{\mu},m} +(1+\gamma_\mu)(DU)^{\dagger}_{m,\mu}\delta_{n,m+\hat{\mu}}] , \tag{20}$$

where

$$DU=U_{\text{new}}-U_{\text{old}}=(V-1)U_{\text{old}}=\left[\sum_{i=0}^{3}C_i\sigma^i\right]U_{\text{old}} . \tag{21}$$

Here $\sigma^i$ are the unit and Pauli matrices. Then we may write $\delta\Delta$ as

$$\delta\Delta=\sum_i C_i\delta\Delta^{(i)} , \tag{22}$$

where $\delta\Delta^{(i)}$ is obtained by replacing $DU$ with $\sigma^i U_{\text{old}}$ in Eq. (20).

In terms of the pseudofermion fields, the connected part of the time-slice propagator is given by

$$\mathcal{G}_c(\tau)=\Gamma_{ij}\tilde{\Gamma}_{kl}\sum_{\substack{x,y\\ x_4-y_4=\tau}}\langle\chi_k^*(y)\phi_j(x)\rangle_{\text{PF}} \times\langle\chi_i^*(x)\phi_1(y)\rangle_{\text{PF}} . \tag{23a}$$

This form, however, is not appropriate to the computation because we should store all the pseudofermion fields generated in the pseudofermionic MC iterations. We can rewrite (23a) as

$$\mathcal{G}_c(\tau)=\Gamma_{ij}\tilde{\Gamma}_{kl}\left[\left\langle\sum_{\substack{x,y\\ x_4-y_4=\tau}}\chi_i^*(x)\phi_j(x)\chi_k^*(y)\phi_l(y)\right\rangle_{\text{PF}}-\sum_{x_4-y_4=\tau}\left\langle\sum_x\chi_i^*(x)\phi_j(x)\right\rangle_{\text{PF}}\left\langle\sum_y\chi_k^*(y)\phi_l(y)\right\rangle_{\text{PF}}\right] . \tag{23b}$$

By this simple trick, we can drastically save computer memory.

### C. Discrete pseudofermions

In this paper we will study the case of a SU(2) gauge theory. We employ for gauge variables the discrete subgroup of SU(2) defined by the symmetries of an icosahedron.[10] Here is a simple trick to reduce the computer time in the pseudofermionic MC calculation: We also make pseudofermion variables discrete. Suppressing Dirac, color, and site indices, we may write the pseudofermion fields as

$$\phi=r\begin{bmatrix}\alpha\\ \beta\end{bmatrix} ,$$

where $\alpha$ and $\beta$ satisfy the condition

$$|\alpha|^2+|\beta|^2=1 .$$

Just this condition is also satisfied by a column vector of an SU(2) matrix. We replace the pseudofermion field $\phi$ by a column vector of the representation of the icosahedral group in the numerical computation.

## III. EXPERIMENT AND DATA

In this experiment we use essentially the same computer program as in our previous paper, where the reliability of the program was discussed in detail. We employ the Metropolis algorithm[11] (not the heat-bath method) for updating both gauge and pseudofermion fields. In the updating process, each link variable is changed by multiplying the old variable times one of the elements closest to the unit element (twelve in the case of the icosahedron). To check the reliability of the program, we have compared[5] $\langle\bar{\psi}\psi\rangle$ of our calculation with that of the hopping-parameter expansion[4] at $k=0.1$, where convergence of the expansion may be very good. The agreement is quite good. Periodic boundary conditions are imposed on both gauge and fermion fields. Two flavors are generated independently to reduce systematic errors. Typical computer time on a $4^4$ lattice is one hour in a VAX 11/780 for one gauge sweep which contains $2\times200$ pseudofermionic MC iterations with five hits. The times for one sweep of the pseudofermion field, for one calculation of $\delta\Delta$ over the fixed pseudofermion, and for one calculation of the propagators are about 7.5, 2.2, and 1.3, respectively, in units of one gauge sweeping time. The rate of acceptance in performing one upgrading step on a pseudofermion vector with four Dirac and two color components is roughly 5%.

Convergence is satisfactorily fast. In Fig. 2 we show the behavior of the expectation value of $S_\phi$ for the first four gauge configurations. The run is initiated with all gauge variables chosen randomly (hot start). For any gauge configuration, the following condition should be satisfied:

$$\langle S_\phi\rangle_{\text{PF}}=(\text{number of degrees of freedom}) . \tag{24}$$

After each gauge sweeping, the pseudofermionic MC calculation starts from the last configuration in the previous iteration. Figure 2 shows that after a few gauge configurations, condition (24) is satisfied with a few percent error. We monitored this quantity when running the program.

The plaquette energy $E_p$ and the chiral order parameter

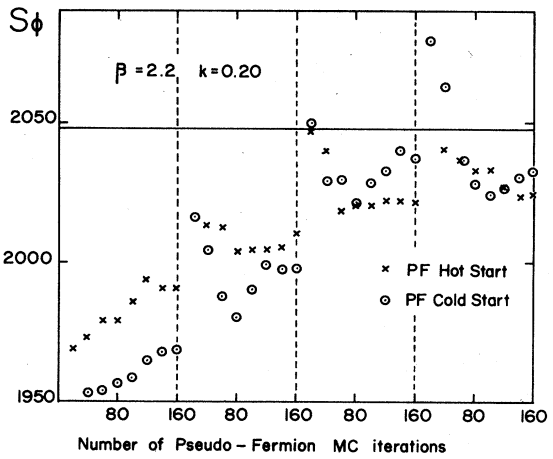


FIG. 2. Expectation value of $S_\phi$ against the number of pseudofermionic MC iterations for the first four gauge configurations. The starting gauge configuration has been chosen randomly (hot start). For each gauge configuration, we have used 40 pseudofermionic MC iterations as thermalization. The crosses correspond to the hot start for the initial pseudofermionic configuration, and the circles to cold start. The theoretical value of $\langle S_\phi \rangle$ is 2048 on a $4^4$ lattice with two color degrees of freedom. After each gauge sweeping, the pseudofermionic MC calculation starts from the last configuration in the previous iteration.

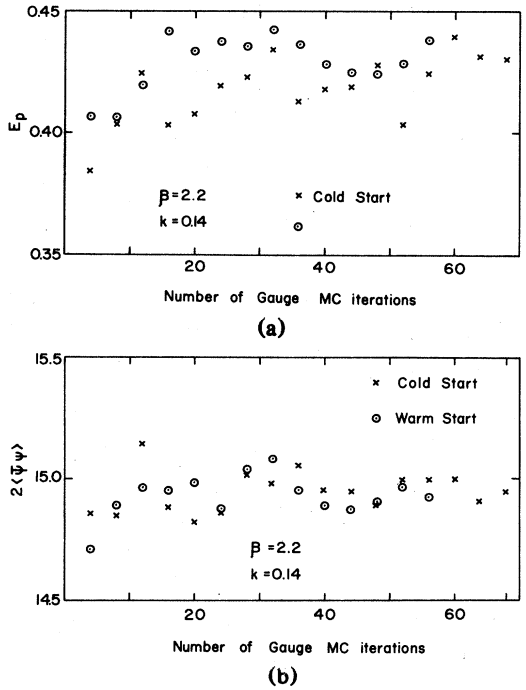


FIG. 3. Expectation values of the plaquette energy (a) and the chiral order parameter $\bar{\psi}(x)\psi(x)$ (b) against the number of MC gauge configurations. Each point was obtained averaging over four gauge configurations. The initial conditions for gauge fields are cold start (crosses) and equilibrium configuration for $\beta=2.2$ and $k=0.18$ (circles), respectively.

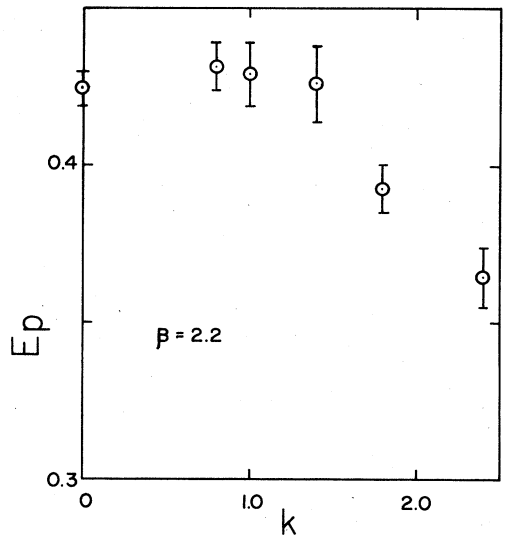


FIG. 4. Expectation value of the plaquette energy as a function of the hopping parameter $k$ ($k=0$ corresponds to the pure gauge case). These values have been obtained from about 50 MC gauge iterations.

$\langle \bar{\psi}\psi \rangle$ are plotted as a function of the number of MC gauge iterations in Fig. 3. Ten or twenty iterations seem to be enough for these quantities to reach equilibrium.

Now we shall report the experimental data. First let us investigate the effects of fermion loops to the gauge fields. In Figs. 4 and 5, we plot the expectation values of the plaquette energy and the Polyakov line as a function of the hopping parameter, where the Polyakov line is defined as[12]

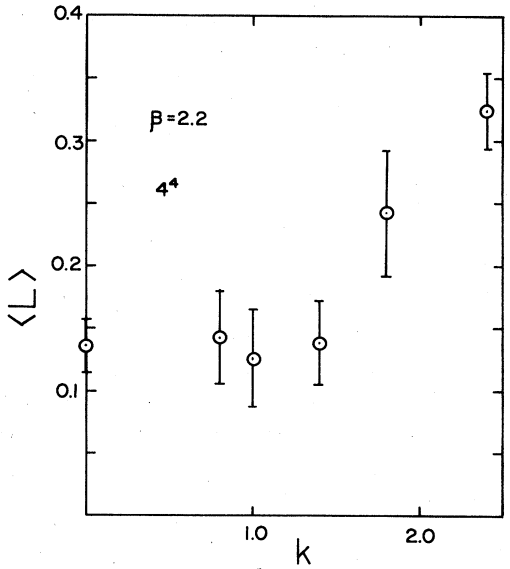


FIG. 5. Expectation value of the Wilson line as a function of the hopping parameter $k$. These values have been obtained under the same conditions as in Fig. 4.

$$L=\frac{1}{n_c}\frac{1}{N^3}\left|\sum_x \mathrm{Tr}\prod_{i=1}^{Nt} U_t(t_i,x)\right| . \quad (25)$$

In the figures the points at $k=0$ correspond to the quenched case, i.e., pure gauge case. When we put quark loops into the system, the plaquette energy decreases, i.e., the system temperature goes down. The Polyakov line is used as an order parameter of deconfinement in the pure gauge theories. Fermion loops increase this order parameter. These observations indicate that fermion loops push the gauge configuration to a more ordered state. The effect becomes prominent above $k\simeq 0.15$. In this region, as we will see, the fermion determinant makes a sizable contribution to the action.

In Fig. 6, we illustrate the fermion-loop effect in the plaquette-plaquette correlation function $G(\tau)$ for $\tau=0$ and 1. We define $G(\tau)$ as

$$G(\tau)=N_s[\langle W(\tau)W(0)\rangle-\langle W(0)\rangle^2] , \quad (26)$$

where

$$W(\tau)=\frac{1}{N_s}\sum_{\substack{\text{spatial}\\ \text{plaquette}}}\tfrac{1}{2}\mathrm{tr}(U_p) ,$$

and $N_s$ is the number of spacelike plaquettes. In this figure, we plot $G(\tau)$ as a function of the number of MC iterations. The solid line and the hatched region in the figures stand for the corresponding values in the pure gauge theory. The value of $G(0)$ is much smaller than that of the pure gauge case: the fluctuation of the plaquette energy decreases due to fermion loops. The value of $G(1)$ is very small and we cannot distinguish it from zero. The pure gauge configurations generated with fermion loops seem to be fairly different from those of the pure gauge case. Note that the glueball masses are essentially determined by $G(\tau)$. Our measurement here does not allow a determination of the glueball masses because of poor statistics and the problem of the fake quark loops due to the small size of the lattice. However, if one wants to know a realistic value of the glueball mass, the effects of fermion loops should be considered seriously.

Next, we will study the problems related to the quark propagators. In Fig. 7, we plot $\langle\bar{\psi}(x)\psi(x)\rangle$ on a $4^4$ lattice as a function of $k$ at $\beta=2.2$. Here $\langle\bar{\psi}(x)\psi(x)\rangle$ is defined by

$$\langle\bar{\psi}(x)\psi(x)\rangle=\frac{1}{n_f N^4}\mathrm{tr}(\Delta^{-1}) .$$

From these values we can estimate the magnitude of $S_{\mathrm{EF}}$ using Eq. (14). We fit the data in Fig. 7 with a spline approximation and integrate it to obtain Fig. 8. We find that there is a sizable contribution of $\det\Delta$ to the total action at large $k$, i.e., light-quark-mass regions.

We have measured $E_p$ and $\langle\bar{\psi}\psi\rangle$ also on a $4^3\times 8$ lattice at $\beta=2.2$. We do not see any significant difference in the data between $4^4$ and $4^3\times 8$ lattices within statistical errors.

In Table I, we present the "masses" of $\pi$, $\rho$, and $\omega$ in reciprocal lattice distance units. Here masses are defined as

$$Ma=\cosh^{-1}\frac{G(\tau=1)}{G(\tau=2)} \text{ [see Eq. (11)]} .$$

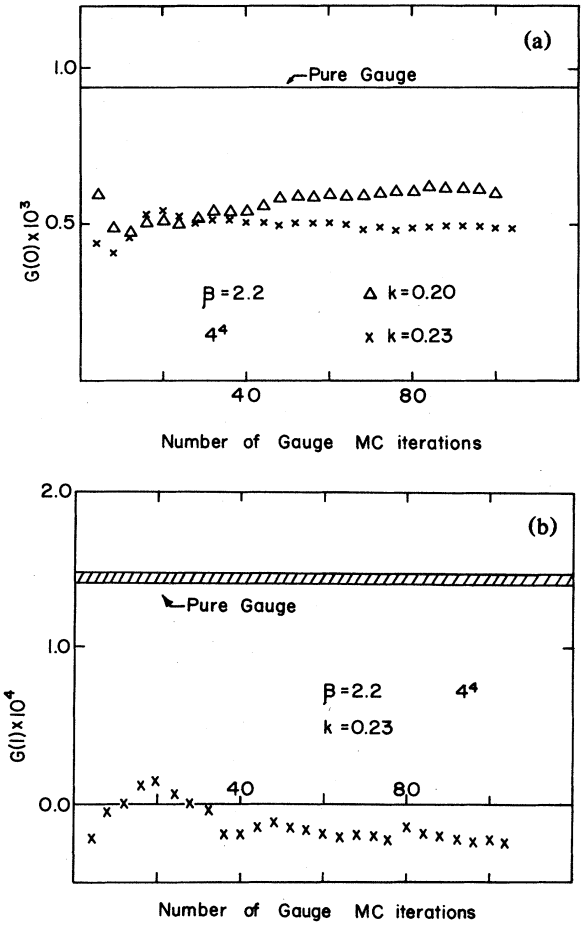


FIG. 6. (a) Time-slice plaquette-plaquette correlation function $G(\tau)$ at $\tau=0$ against the number of MC gauge sweeps. The solid line stands for the pure gauge case. The triangles correspond to $k=0.20$ and have been obtained with a thermalization of 40 gauge MC iterations. The crosses correspond to $k=0.23$ and the thermalization is 68 sweeps. (b) Time-slice plaquette-plaquette correlation function $G(\tau)$ at $\tau=1$ against the number of MC gauge sweeps. The hatched region stands for the corresponding value in the pure gauge case. The crosses correspond to $k=0.23$ and the thermalization for gauge fields is 68 sweeps.

We have found that the $\pi/\rho$ mass ratios are about 1 and that the splitting of $\rho$ and $\omega$ has the correct sign for the observed region of the parameters. We should notice, however, that (i) the mass defined above has a strong contamination of higher states because of the short distance of the propagators; (ii) the value of the Polyakov line is larger than that of the quenched case and the finite-temperature effects are more serious; (iii) in this experiment we could not determine the physical $k$ (fixed for example from $\pi$-$\rho$ mass difference) at which all hadronic quantities should be measured; and (iv) statistics is not enough.

Recently, Otto[13] has claimed that even a small number of pseudofermionic iterations might be sufficient in order

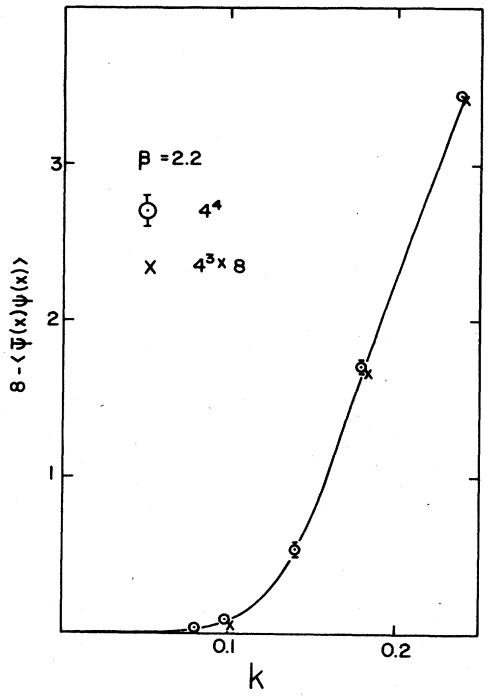


FIG. 7. Expectation value per flavor of $8-\langle\bar{\psi}(x)\psi(x)\rangle$ as a function of the hopping parameter $k$. The solid line is a spline interpolation for the data on a $4^4$ lattice. The crosses are the corresponding expectation values in a $4^3\times 8$ lattice.

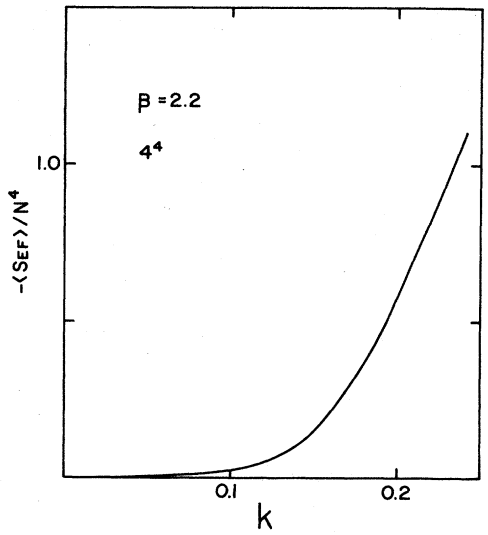


FIG. 8. Expectation values of $S_\phi$ as a function of the hopping parameter $k$ and for one flavor. This figure was obtained by integrating Eq. (13) and using the values of $\langle\bar{\psi}\psi\rangle$ represented in Fig. 7.

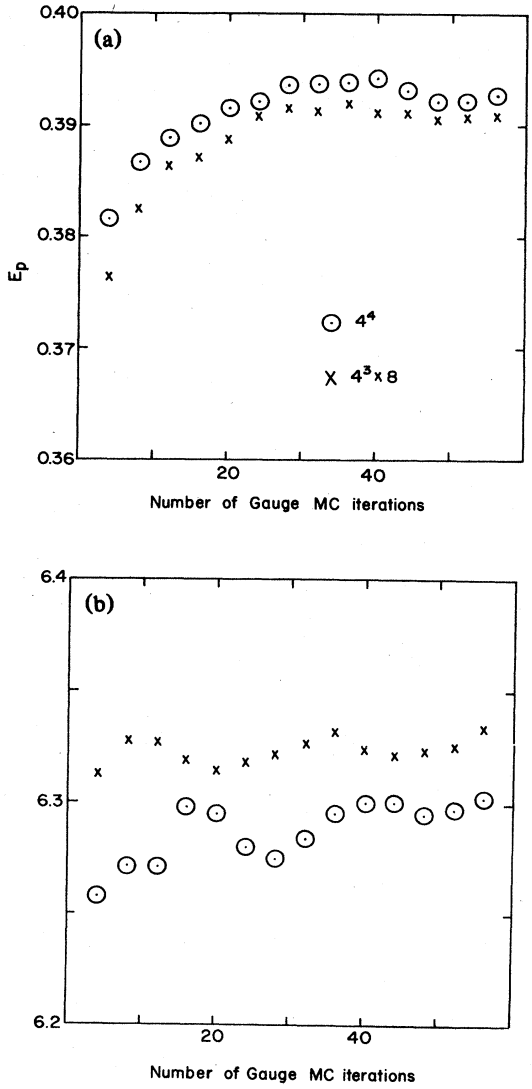


FIG. 9. Expectation values of mean energy per plaquette, $E_p$, (a) and chiral order parameter $\bar{\psi}\psi$ (b) against the number of MC gauge sweeps. The circles have been obtained from a $4^4$ lattice and the crosses are the results for a $4^3\times 8$ lattice.

to include fermion loops. We have performed two experiments with the same conditions except the number of MC iterations (experiments 2a and 2b in Table I). Though the values of hadron masses obtained from these two experiments are consistent with each other, the error bars of experiment 2b are much larger than those of experiment 2a as a natural consequence of the smaller number of pseudofermionic iterations. Both experiments give about the same value of $\langle\bar{\psi}\psi\rangle$. This is also the case for the plaquette energy: $E_p=0.293$ for experiment 2a and $E_p=0.310$ for experiment 2b. These quantities can be usually obtained with small statistical error. For such quantities, a smaller number of pseudofermionic iterations might be sufficient if we include the proper number of thermalization runs.

TABLE I. Column 1 contains the conventional line number assigned for identification of the different runs; column 2 contains the values of $\beta$, column 3 those of $k$, the hopping parameter. Column 4 contains the size of the lattice. Column 5 contains the average of $\langle\bar{\psi}\psi\rangle$ over the sample expressed by columns 9 and 10. All the values in column 5 fluctuate typically inside seven percent. Columns 6, 7, and 8 contain the masses of the hadrons $\pi$, $\rho$, and $\omega$, respectively, measured in reciprocal of the lattice spacing for the experiments where they have been measured. The errors take into account the statistical correlation (Ref. 18). In particular, for the propagators at $\tau=2$, no correlation between consecutive groups of four gauge iterations has been found. We have estimated the error of the latter by the differences between the averages of the odd and even groups of four consecutive measurements. From this and the correlation-connected error (Ref. 19) for the propagators at $\tau=1$, a typical error for the masses has been estimated at $\pm 0.60$ in reciprocal lattice spacings. For the errors in row 2b, which are very large, the statistical correlation has not been considered. Column 9 contains the number of thermalization gauge sweeps, followed by the number of sweeps on which the averages have been evaluated. Analogously, column 10 contains, for each flavor ($2\times$) the number of thermalization pseudofermion sweeps, followed by the number of sweeps on which averages are evaluated. The initial conditions for the different lines are the following: (1) Random configuration (hot start). (2a) Hot start. (2b) A late configuration from 3. (3) Last configuration from 2. (4) A late configuration from 3. (5) Last configuration from 3. (6) Last configuration from 5. (7) Last configuration from 6. (8) Last configuration from 7. (9) Last configuration from 8. (10) Cold configuration (all link variables set to 1). (11) Last configuration from 10. (12) Last configuration from 11.

| No. | $\beta$ | $k$ | Size | $\langle\bar{\psi}\psi\rangle$ | $m_\pi a$ | $m_\rho a$ | $m_\omega a$ | Number of gauge sweeps | Number of Fermi sweeps |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 3.0 | 0.23 | $4^4$ | 4.67 | 3.14 | 2.69 | 2.82 | 8 + 128 | $2\times(25+175)$ |
| 2a | 2.5 | 0.23 | $4^4$ | 4.75 | 2.09 | 2.75 | 3.47 | 12 + 144 | $2\times(25+175)$ |
| 2b | 2.5 | 0.23 | $4^4$ | 4.73 | 1.90±1.19 | 2.11±0.42 | 2.84±2.72 | 20 + 200 | $2\times(5+15)$ |
| 3 | 2.2 | 0.23 | $4^4$ | 4.82 | 2.28 | 2.46 | 2.61 | 28 + 204 | $2\times(25+175)$ |
| 4 | 2.2 | 0.20 | $4^4$ | 5.70 | 2.62 | 2.28 | 2.45 | 4 + 168 | $2\times(25+175)$ |
| 5 | 2.2 | 0.24 | $4^4$ | 4.50 | | | | 4+52 | $2\times(25+25)$ |
| 6 | 2.2 | 0.18 | $4^4$ | 6.30 | | | | 4+52 | $2\times(25+25)$ |
| 7 | 2.2 | 0.14 | $4^4$ | 7.46 | | | | 4+40 | $2\times(25+25)$ |
| 8 | 2.2 | 0.10 | $4^4$ | 7.92 | | | | 4+52 | $2\times(25+25)$ |
| 9 | 2.2 | 0.08 | $4^4$ | 7.97 | | | | 4+72 | $2\times(25+25)$ |
| 10 | 2.2 | 0.24 | $4^3\times 8$ | 4.57 | | | | 4+48 | $2\times(25+25)$ |
| 11 | 2.2 | 0.18 | $4^3\times 8$ | 6.34 | | | | 4+54 | $2\times(25+25)$ |
| 12 | 2.2 | 0.10 | $4^3\times 8$ | 7.93 | | | | 4+64 | $2\times(25+25)$ |

## IV. DISCUSSIONS

The experiment presented in this article demonstrates, we believe, that we can and we should proceed in the MC simulation of gauge theories with dynamical fermions and that, on the way, many things should be clarified. We hope that one can make the best use of the experiences here at the next steps. Though the small size of the lattice and the employment of SU(2) as gauge group are strong limitations in this experiment, the following observations made here seem to be general features.

(i) The CPU time is not hopelessly long.

(ii) The gauge configurations generated with light quark loops are fairly different from those of the pure gauge case.

(iii) There is no strong size effects between $4^4$ and $4^3\times 8$ lattices in regard to $E_p$ and $\langle\bar{\psi}\psi\rangle$.

(iv) The $E_p$ and $\langle\bar{\psi}\psi\rangle$ do not suffer too much from statistical errors, but the hadron propagators do.

Let us comment upon these points. We have used several tricks to save computer time, but reduction of CPU time is still possible.[14] We employed the Metropolis algorithm for the pseudofermionic MC calculation. However, the heat-bath method could be more efficient because this algorithm works well for a Gaussian distribution. We have used here the standard Wilson action with the Wilson term $r$ set to 1. If we want to study only the global nature of the fields (the plaquette energy, the Polyakov line, $\langle\bar{\psi}\psi\rangle$, etc.) and give up the calculation of $\Delta^{-1}$, we can perform simulations in less CPU time with the Kogut-Susskind action because it has one component on each site, though it is not clear whether a lattice with the Kogut-Susskind action is equivalent to a lattice of the same size with the Wilson action.

In the case of the quenched approximation, there is a window where the correlation length is large enough so that scaling has set in and yet not so large compared to the lattice size.[15] The data described in the previous section suggest that the correlation length changes when the fermion loops are considered. The lattice distance is also different from that of the pure gauge theories. In the scaling region, the lattice distance is related to the bare coupling constant $g$ as

$$a=\frac{1}{\Lambda}(\beta_0 g^2)^{-\beta_1/2\beta_0^2}\exp\left[-\frac{1}{2\beta_0 g^2}\right], \tag{27a}$$

where $\beta_0$ and $\beta_1$ are the coefficients of the first and the second terms of the $\beta$ function and, for massless QCD, they are given by[16]

$$\beta_0=\frac{1}{(4\pi)^2}\left(\tfrac{11}{3}n_c-\tfrac{2}{3}n_f\right),$$
$$\beta_1=\frac{1}{(4\pi)^2}\left[\tfrac{34}{3}n_c{}^2-\tfrac{10}{3}n_cn_f-\frac{1}{n_c}(n_c{}^2-1)n_f\right]. \quad (27b)$$

From this formula we can see that our lattice ($n_c=2$, $n_f=2$) shrinks faster than that with $n_f=0$ as $\beta(=4/g^2)$ increases. This may be part of the reason why the expectation values of the Polyakov line are larger than in the pure gauge case. We should search for a new window and remeasure the correlation length, the glueball masses, etc., there.

The quantities $E_p$ and $\langle\bar{\psi}\psi\rangle$ do not suffer much from statistical errors and are stable against changing the lattice size. The estimation of the fermion determinant in Fig. 8 is reliable. Convergence of $E_p$ and $\langle\bar{\psi}\psi\rangle$ even on a $4^3\times 8$ lattice is good (see Fig. 9). This raises our hope of going to larger lattices.

As we have seen in this experiment, the field configuration on a lattice with quark loops is fairly different from that of the quenched approximation. In the latter case, Kogut *et al.* and the Bielefeld group have shown that at finite temperature the system presents a deconfinement phase where chiral symmetry is restored. With quark loops, however, the situation may be very different because the phase transition between confined and deconfined phases disappears if we use the Polyakov line as an order parameter.[17] Furthermore, the gauge configurations which give zero eigenvalues of $\Delta$ being essential to the chiral symmetry breaking, are suppressed with respect to the quenched case due to the measure $\det\Delta$. This problem should be investigated very urgently.

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[1]H. Hamber and G. Parisi, Phys. Rev. Lett. **47**, 1792 (1981); Phys. Rev. D **27**, 208 (1983); E. Marinari, G. Parisi, and C. Rebbi, Phys. Rev. Lett. **47**,1795 (1981); D. Weingarten, Phys. Lett. **109B**, 57 (1982); Nucl. Phys. **B215**, 1 (1983); F. Fucito *et al.*, *ibid.* **B210** [FS6], 314 (1982); G. Martinelli, G. Parisi, R. Petronzio, and F. Rapuano, Phys. Lett. **116B**, 434 (1982); C. Bernard, T. Draper, K. Olynyk, and M. Rushton, Phys. Rev. Lett. **49**, 1076 (1982).

[2]A. Hasenfratz, P. Hasenfratz, Z. Kunst, and C. B. Lang, Phys. Lett. **117B**, 81 (1982); P. Hasenfratz and I. Montvay, Phys. Rev. Lett. **50**, 309 (1983); H. Lipps, G. Martinelli, R. Petronzio, and F. Rapuano, Phys. Lett. **126B**, 250 (1983); P. Hasenfratz and F. Montvay, Nucl. Phys. **B237**, 237 (1984); M. Fukugita, T. Kaneko, and A. Ukawa, *ibid.* **B230** [FS10], 62 (1983).

[3]J. Kogut *et al.*, Phys. Rev. Lett. **48**, 1140 (1982); **50**, 393 (1983); J. Engels, F. Karsch, and H. Satz, Phys. Lett. **113B**, 398 (1982); J. Engels and F. Karsch, *ibid.* **125B**, 481 (1983). See also H. Hamber and G. Parisi in Ref. 1.

[4]O. Stamatescu, Phys. Rev. D **25**, 1130 (1982); C. B. Lang and H. Nicolai, Nucl. Phys. **B200** [FS4], 135 (1982); A. Hasenfratz, P. Hasenfratz, Z. Kunst, and C. B. Lang, Phys. Lett. **110B**, 289 (1982); P. Hasenfratz, in *Lattice Gauge Theories, Supersymmetry, and Grand Unification,* proceedings of the 6th Johns Hopkins Workshop on Current Problems in Particle Theory, Florence, 1982 (Physics Department, Johns Hopkins University, Baltimore, 1982). See also J. Kuti and J. Polony, *ibid.*, where the hopping-parameter expansion series was calculated by a subtle stochastic method. To our knowledge, this is the first paper which studied the effect of quark loops positively.

[5]V. Azcoiti and A. Nakamura, Phys. Rev. D **27**, 2559 (1983).

[6]K. Wilson, in *New Phenomena in Subnuclear Physics,* proceedings of the 14th course of the International School of Subnuclear Physics, Erice, 1975, edited by A. Zichichi (Plenum, New York, 1977).

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

[8]T. Banks *et al.*, Phys. Rev. D **15**, 1111 (1977); L Susskind, *ibid.* **16**, 3031 (1977).

[9]F. Fucito, E. Marinari, G. Parisi, and C. Rebbi, Nucl. Phys. **B180**, 369 (1981); E. Marinari, G. Parisi, and C. Rebbi, *ibid.* **B190** [FS3], 734 (1981).

[10]C. Rebbi, Phys. Rev. D **21**, 3350 (1980); D. Petcher and D. H. Weingarten, *ibid.* **22**, 2465 (1980).

[11]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).

[12]A. N. Polyakov, Phys. Lett. **72B**, 477 (1978); N. Weiss, Phys. Rev. D **24**, 475 (1981); L. G. Yaffe and B. Svetitsky, *ibid.* **26**, 963 (1982); G. Martinelli, G. Parisi, R. Petronzio, and F. Rapuano, Phys. Lett. **122B**, 283 (1983).

[13]S. Otto and M. Randeria, Nucl. Phys. **B220**, 479 (1983); B. S. Otto, Phys. Lett. **135B**, 129 (1984).

[14]See G. Parisi, Frascati Report No. LNF-84/14, 1984 (unpublished), where strategies and tactics to reduce CPU time and memories are discussed from many points of view.

[15]M. Creutz, L. Jacobs, and C. Rebbi, Phys. Rev. Lett. **42**, 1390 (1979); Phys. Rev. D **20**, 1915 (1979); M. Creutz, Phys. Rev. Lett. **43**, 553 (1979); Phys. Rev. D **21**, 2308 (1980).

[16]See, for example, C. Itzykson and J. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980), Chap. 13.

[17]P. Hasenfratz, F. Karsch, and I. O. Stamatescu, Phys. Lett. **133B**, 221 (1983); A. Nakamura (unpublished).
[18]T. A. DeGrand and D. Toussaint, Phys. Rev. D **22**, 2478 (1980).
[19]L. D. McLerran and B. Svetitsky, Phys. Rev. D **24**, 450 (1981).