JUN 1 2 1987

BROOKHAVEN NATIONAL LABORATORY

CONF-8609142--4

February 1987

BNL-39764

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ABSTRACT

We present our preliminary results of a pseudofermion simulation of QCD, on a $10^3 \cdot 32$ lattice at $\beta = 5.7$. The fermions are of the Kogut-Susskind type (3 flavors) with mass $ma = 0.05$. It is found that the hadron propagators take more than 10000 Metropolis iterations to equilibrate, a factor 5 more than what is needed in a typical quenched calculation. We present also our results on the effects of dynamical quarks on the Wilson loops.

* Talk given by J. Potvin at Lattice Gauge Theory '86, BNL, 14-19 September 1986, to be published in the Proceedings.

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ABSTRACT

We present our preliminary results of a pseudofermion simulation of QCD, on a $10^3 \cdot 32$ lattice at $\beta = 5.7$. The fermions are of the Kogut-Susskind type (3 flavors) with mass $ma = 0.05$. It is found that the hadron propagators take more than 10000 Metropolis iterations to equilibrate, a factor 5 more than what is needed in a typical quenched calculation. We present also our results on the effects of dynamical quarks on the Wilson loops.

MOTIVATIONS

The calculation of the hadron mass spectrum without including the dynamical quarks (i.e. the quenched approximation) has lead to very encouraging results. For one, the calculated hadron masses have been found consistent with the experimental values, within statistical and systematic error. Also, the breaking of chiral symmetry and the Goldstone nature of the pion have been seen.¹

Of course, the quenched approximation is not the whole story, since QCD is a theory about gluons AND quarks. It is therefore important to verify that, upon the re-introduction of the dynamical quarks into the picture, the above results will not change much. Moreover, dynamical quark effects should be visible in the heavy quark potential, at separations beyond one Fermi where hadronization takes place.

It has been known for a long time that the unquenched simulation of QCD is much more demanding on computer resources. It is only with the recent availability of supercomputer time that algorithms with dynamical fermions have for the first time been tried out and tested on reasonably large lattices ($\geq 8^4$) and couplings (≥ 5.0), and with small masses (≤ 0.10). Examples of such algorithms are presented and discussed in this Conference Proceedings.

Most physics applications of these algorithms have been concerned with QCD at finite temperature. In contrast, only three large scale studies of the hadron-mass spectrum have been carried out:

1. a Langevin calculation by Fukugita et al.² on a $9^3 \cdot 18$ lattice, at $\beta = 5.5$ with Wilson fermions. For more details, see Fukugita's talk in these Proceedings.
2. a pseudofermion simulation by Fucito et al.,³ on a $12^3 \cdot 24$ lattice at $\beta = 5.4$ with three flavors of Kogut-Susskind fermions. Three mass values were tried: 0.02, 0.05, and 0.10. Their statistics was limited however, with only nine propagators per mass.
3. another pseudofermion calculation, by Laerman et al.,⁴ this time with the group SU(2). The lattice size was $8^3 \cdot 16$ and $1.85 \leq \beta \leq 2.50$; four flavors of Kogut-Susskind fermions were used in the mass range $.035 \leq ma \leq 0.200$.

We have continued this exploratory effort with another pseudofermion calculation, at mass $ma = 0.05$ with three flavors of Kogut-Susskind quarks. The lattice size was $10^3 \cdot 32$, at $\beta = 5.7$. In this talk I will present our preliminary results with emphasis on the equilibrium time required for the Wilson loops ($W(1,1)$) and pion propagator (P_{π_0}). Our conclusions will be that it is very different for both quantities: thousands more iterations (i.e. link upgrades) are needed for $W(1,1)$ than for P_{π_0} ; this is also many more than what is required in a calculation of P_{π_0} in the quenched approximation.

Our simulation was carried out on a CDC CYBER 205 based at Rockville Md., thanks to the generosity of the Control Data Corporation.

THE ALGORITHM

According to the procedure described in Ref. 5 and Ref. 6, the pseudo-fermions ϕ_x are upgraded first with a heat bath algorithm in the background of fixed gauge fields. Here the ϕ_x are modified in the following way,

$$\begin{aligned}\phi_x' &= \phi_x + \delta\phi_x \\ \delta\phi_x &= \frac{1}{\sqrt{2+m^2}}V_x + \frac{1}{2+m^2} \left(D^\dagger + m \right) (D + m) \phi_x\end{aligned}\quad (1)$$

V_x being a Gaussian random number of unit variance and $(D + m)$ the Dirac operator. Such an upgrade is done 300 times, calculating and accumulating the reaction J_x^μ every 12 sweeps. J_x^μ is needed in the calculation of the variation of the total action Ref. 6:

$$\delta S = \delta S_{\text{Gauge}} - \frac{1}{8} n_f \sum_{x,\mu} (Tr \langle J_x^\mu \rangle \delta U_x^\mu + \text{H.C.}) \quad (2)$$

$\langle J_x^\mu \rangle$ is thus evaluated from a sample of 25 values, in similarity with the calculations of Ref. 3 and Ref. 7. A distinct feature of our study is that not all ϕ_x are upgraded at each pseudofermion sweep but only a subset of approximately 1000, chosen in a uniformly random fashion (the sites being still distanced at least 3 steps away to allow for vectorization). This procedure still satisfies detailed balance, and eliminates any potential directional correlations due to upgrading. With the use of asynchronous I/O, it also shortens the pseudofermion upgrade while maintaining a reasonable vector length.

After the 300 pseudofermion sweeps, the link variables are then upgraded with a standard Metropolis procedure, at a rate of 8 upgrades per link. Here the acceptance is 81%. This coupled heat bath/Metropolis update (or "iteration") took 0.3 milliseconds per link and was run for a total of 9000 iterations (14500 after this Meeting). The Wilson loops were measured every 10 iterations and propagators every 500.

WILSON LOOPS

Figures 1 and 2 show the evolution of the 1×1 , 2×2 , 3×3 and 4×4 Wilson loops with respect to iteration number. Clearly, the smaller loops have equilibrated after 2500 iterations, more or less. The larger ones are of course slower and show equilibration after 4000 iterations.

After 14500 iterations, we get

$$W(1,1) = 0.5816 \pm .0002 \quad (3)$$

Fig. 1: 1×1 and 2×2 Wilson loops versus the iteration number.

Fig. 2: 3×3 and 4×4 Wilson loops versus the iteration number.

Fig. 3: Comparison of quenched and unquenched Wilson loops.

to be compared with the quenched value at the same coupling.⁸

$$W(1,1) = 0.5490 \pm .0010 \quad (4)$$

By running a quenched simulation on the same lattice, we have found that the value shown in (3) is reproduced within errors at $\beta = 5.89$. Let us mention finally that a recent study by Gai, Gocksch and Heller⁹ suggests that the pseudofermion algorithm may underestimate $W(1,1)$ at $ma = 0.05$.

Figure 3 is a comparison of unquenched Wilson loops at $\beta = 5.7$ and quenched ones at 5.89. It demonstrates that the effects of the dynamical fermions cannot be absorbed into a simple renormalization of β , m , or n_f . This confirms early claims by Gai and Karsch¹⁰ ($ma = 0.10$). Let us point out however that on this issue Fukugita et al.² have concluded otherwise.

HADRON PROPAGATORS

The hadron propagators are defined by³

$$\text{meson} : P_{tt_0}^{m(k)} = \sum_x S_x^k \text{tr} \Delta_{(x,t)}^{-1} \Delta_{(x,t_0)}^{-1} \quad (5)$$

$$\text{baryon} : P_{tt_0}^{b(k)} = \sum_x S_x^k \det \Delta^{-1} \quad (6)$$

$$\Delta(x, t_0) = (D + \tilde{m}a)_{x,t_0} \quad (7)$$

The matrix Δ was inverted with the conjugate gradient algorithm in the following parameter range:

$\tilde{m}a$	C-G sweeps	residue (Barkai et al.[1])
.50	50	10^{-8}
.10	100	10^{-7}
.05	200	10^{-7}
.02	350	10^{-6}
.01	500	10^{-6}

Figure 4 shows how the pion propagator P_{tt_0} evolves with the (Metropolis) iteration number, for $\tilde{m}a = .05$ and $\tilde{m}a = .01$. Each continuous line approximates the general path followed by the data as it migrates through the time slices, during a given iteration. This data is averaged over three source points ("t₀").

The figure shows the propagator near $t = 16$ to decrease by an order of magnitude over a range of at least 6000 iterations. Not surprisingly, the effect is more pronounced at $\tilde{m}a = .01$. In that case, 10000 are needed to get a good idea of how far down the minimum of P_{tt_0} has to go. Not shown is the fact that it does go up again, from iteration 10000 to 14500, without going beyond the 3000 line (this data was generated after this Lattice Meeting). In the case $\tilde{m}a = .05$, we need 6000 iterations to see the minimum go down and up again (fig. 4).

All this shows that one needs at least several thousands iterations to get a good idea of the drift of propagator values through the simulation. This is many more iterations than for $W(1,1)$. It is also many more than the 2000 commonly used in most previous quenched studies. We have verified this last point ourselves in our quenched runs at $\beta = 5.89$ (fig. 5).

In the parameter range $ma \approx .05$ and $\tilde{m}a = .01, .05$, it appears that a pseudofermion calculation of the hadron mass spectrum with good

Fig. 4: The unquenched pion propagator. (a) $\tilde{m}a = .05$ and (b) $\tilde{m}a = .01$.

Fig. 5: The quenched pion propagator. (a) $\tilde{m}a = .05$ (b) $\tilde{m}a = .01$.

statistics requires at least 4 to 5 times more iterations than in the quenched case. This is because a pseudofermion simulation has one more $(D + ma)$ -inversion, which will also be affected by critical slowdown caused by small m .

Fig. 6: The unquenched π and ρ propagators.

Figure 6 shows the resulting π and ρ unquenched propagators. The mass can be extracted according to standard methods; figure 7 displays preliminary pion masses, as function of $\sqrt{\tilde{m}_q a}$. The full analysis will be presented elsewhere.

Fig. 7: Pion masses (unquenched).

CONCLUSIONS

To the best of our knowledge, this is the first demonstration of critical slow down of long wavelength structures in a background of dynamical fermions. Our propagators at $\tilde{m}a = ma = .05$ certainly need more than 8000 iteration on a $10^3 \cdot 32$ lattice in order to get reasonably good statistics. In the case of $ma = .05$ $\tilde{m}a = .01$ the outlook is worse, as at least 10000 to 14500 are needed. This indicates how hard a similar study at $ma = \tilde{m}a = .01$ will

be (we anticipate a factor 2 in iteration number). Compared with a quenched calculation, this represents 4 to 5 times more iterations, a hefty 40 to 50-fold increase in computer time, if a factor of 0.1 is assumed for link upgrade in a quenched simulation.

This makes the importance of acceleration of long wavelength structures equilibration time all too obvious. Let us mention that this question has already been addressed by the Cornell¹¹ and the Kyoto-Tsukuba¹² groups in the context of the Langevin equation.

The situation looks better in the case of Wilson loops, where 3000 or so iterations are required for equilibration. We have studied the $Q\bar{Q}$ -potential and found that the effects of dynamical fermions do not amount to a simple renormalization of the parameters.

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