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# Comparison of an Exact Fermion Monte Carlo Algorithm with the Pseudofermion Method Using Staggered Fermions

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We present first results obtained from a simulation of lattice QCD with staggered fermions by a Monte Carlo algorithm that incorporates the effect of the fermion determinant *exactly*. The chiral condensate $\bar{\chi}\chi$ and various Wilson-loop expectation values are measured on a $4^4$ space-time lattice and the results are compared with the same quantities measured on the same-size lattice with the pseudofermion method. A quantitatively good agreement is found.

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Numerical simulations of lattice QCD have led us to a lot of interesting results. An outstanding problem in this field has been the proper inclusion of the fermion determinant. In fact, all the early calculations were done in the quenched approximation, i.e., without the determinant. Recently a tremendous effort by various groups has gone into the development of new fermion algorithms, as well as into the application of older, more established algorithms to problems in both finite-temperature lattice QCD and hadron spectroscopy. Among the latter, the ones that have been studied the most are the pseudofermion[1] and the microcanonical method.[2] Both algorithms have been applied extensively to the simulation of finite-temperature QCD[3,4] and the results that were obtained are in qualitative agreement with the expectations one has for the phase structure of the theory. Furthermore there is evidence for a *quantitative* agreement between the two methods.[5]

Both of the above methods have obvious shortcomings. The microcanonical method for one is based on the crucial assumption of ergodicity. If for some reason (a hidden symmetry, for example) the system only explores a finite portion of phase space, the results obtained could be wrong. On the other hand, the pseudofermion method explicitly violates detailed balance. This violation can be kept small by choosing a small step size in the gauge-field update (large acceptance) and a large number of pseudofermionic hits.

An improved version of the microcanonical method has been presented recently.[6] The basic idea is to "refresh" the conjugate momenta occasionally so as to build into the method an element of randomness that the original, fully deterministic one does not have. However, this algorithm also faces one problem common to all algorithms.[7] The long- and short-wavelength modes do not tend to equilibrate at the same rate, but it takes the long-wavelength modes longer by a factor proportional to the inverse bare-quark mass squared. Batrouni *et al.*,[8] in their study of an algorithm based on the Langevin equation, show how one might be able to avoid this problem by the use of Fourier acceleration methods. This approach looks very promising and can in principle be applied to any method that is based on the solution of a differential equation.

In the implementation of the pseudofermion method the problem of different rates of convergence at different length scales has up to now not been specifically addressed. However, the method is so effi-

cient that the hope is that by just running long enough one would achieve equilibration on *all* scales. For this to be true one must, however, tune the two crucial parameters of the method, the number of pseudofermionic hits and the acceptance rate, to values which amount to a maximum *permissible* violation of detailed balance. A question, however, immediately comes to mind: How do we know that for those values of the parameters all expectation values will converge to their true values? A similar question also needs to be answered in the case of the algorithms based on the solution of differential equations. One discretizes these equations in order to solve them on the computer. The size of the smallest step in the (fictitious) time direction governs the convergence there.

In this Letter we present the results of our attempt to answer these important questions. We have written a program that takes into account the effect of the fermion determinant exactly. The hope is that discrepancies in the expectation values of observables in a comparison will help in restricting the allowed ranges of the parameters of other methods. As an illustrative example, we will consider the pseudofermion algorithm here. This idea is not new, to be sure; as a matter of fact the algorithm used in the present paper is that used by Otto.[9] However, there as well as in Ref. 7 Wilson fermions were used and the lattice size was only $2^4$, resulting in a smaller number of observables to compare. Our results have been obtained on a $4^4$ lattice and we measured $\bar{\chi}\chi$ and all the planar Wilson loops up to the linear dimension 3. While our lattice size is still quite small compared to those employed in realistic calculations, we believe it suffices for at least the smaller Wilson loops such as the plaquette in the sense that our results should already be quite close to the infinite-lattice limit. The data presented here are in a sense preliminary. A complete study would involve investigation of the stability of the results with respect to the various parameters involved in both the exact algorithm and the other approximate ones such as the pseudofermion method. Such an investigation is being pursued presently and the detailed results will be published soon.[10] It is hoped that the results of these studies will set a benchmark with which all other fermion algorithms employing staggered fermions can be compared.

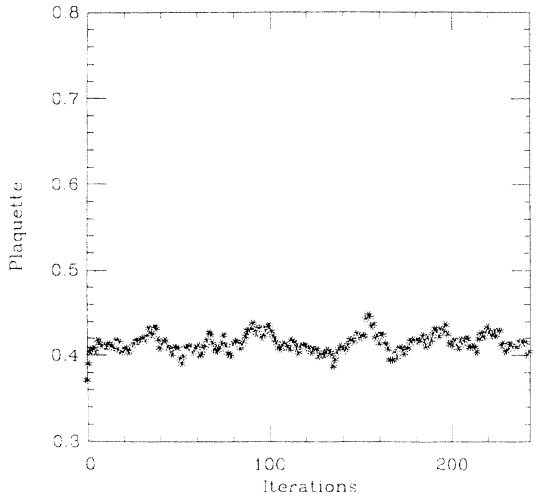


FIG. 1. Evolution of the average plaquette by the exact algorithm. The gauge-field coupling $\beta$ is 4.8.

The basic idea of the exact algorithm goes back to Scalapino and Sugar[11] who realized in the context of two-dimensional models that the problem of calculating the fermionic determinant can be reduced to calculating the determinant of a rather small matrix. Here we want to generate an ensemble of configurations in which the probability of a configuration is given by the exponential of its action

$$S=(\beta/2N)\sum_P(\mathrm{tr}\,U_P+\mathrm{H.c.})+S_F, \tag{1}$$

where $S_F$ is given by

$$S_F=\tfrac{1}{2}\sum_{x,y,\mu}\eta_\mu(x)\bar{\chi}(x)[U_\mu(x)\delta_{x,y-\mu}-U_\mu^\dagger(y)\delta_{x,y+\mu}]\chi(y)+\sum_x m\bar{\chi}(x)\chi(x). \tag{2}$$

Our notation is a fairly standard one. Integrating out the fermion fields in (2) leads to the determinant of the lattice Dirac operator which we will from now on call $M_{x,y}$, supressing the color indices. In the numerical simulations using the conventional Metropolis algorithm what is needed is the quantity

$$e^{-\delta S}=\det(1+M^{-1}\delta M)e^{-\delta S_G}. \tag{3}$$

In (3) $\delta M$ is the change in $M$ under a change $\delta U_\mu(x)$ in the link variable $U_\mu(x)$. After a little algebra one easily obtains the following expression for the determinant ratio in (3):

$$\det\begin{pmatrix}1-\frac{1}{2}\eta_\mu(x)M^{-1}_{x,x+\mu}\delta U_\mu^\dagger(x) & \frac{1}{2}\eta_\mu(x)M^{-1}_{x,x}\delta U_\mu(x)\\ -\frac{1}{2}\eta_\mu(x)M^{-1}_{x+\mu,x+\mu}\delta U_\mu^\dagger(x) & 1+\frac{1}{2}\eta_\mu(x)M^{-1}_{x+\mu,x}\delta U_\mu(x)\end{pmatrix}. \tag{4}$$

TABLE I. Summary of our data. (Exact algorithm.)

| $W(1,1)$ | $W(1,2)$ | $W(1,3)$ | $W(2,2)$ | $W(2,3)$ | $W(3,3)$ | $\bar{\chi}\chi/3$ |
|---|---|---|---|---|---|---|
| 0.415 | 0.177 | 0.074 | 0.035 | 0.008 | −0.001 | 0.4018 |
| (0.003) | (0.003) | (0.003) | (0.003) | (0.002) | (0.002) | (0.006) |

It should be clear from the above discussion that for every attempted Metropolis hit for a link variable we have to calculate, taking into account color, the determinant of a $6\times6$ matrix. To obtain the matrix elements of the inverse fermion propagator needed in (4) we chose to calculate six columns of the inverse using the conjugate-gradient algorithm. Clearly this is a very time-consuming method, but it is also known to have a better convergence[12] irrespective of the value of the quark mass. Note, however, that no approximations were made. In particular, the magnitude of $\delta U_\mu$ is arbitrary. The algorithm can be made more efficient by doing multiple Metropolis hits per link without much cost in computer time. It is easy to show that we only need to know the inverse of the $6\times6$ matrix appearing in (4) in order to compute the new columns of $M^{-1}$ from the old ones after a change in $U_\mu$ has been accepted. We also used the conjugate-gradient method for this purpose.

In our simulation eight Metropolis hits per link were done. On our $4^4$ lattice this procedure took ten minutes per sweep through the lattice, with most of the time spent finding the columns of the inverse using the conjugate-gradient algorithm. The average acceptance per hit was around 43%.

Here we compare simple expectation values calculated with the exact algorithm and the pseudofermion method.[1] The method corresponds to expanding the determinant ratio (3) in powers of $\delta U_\mu$ and keeping only terms linear in this quantity. The great advantage of this method is that $M^{-1}$ must only be calculated *once for each sweep* through the lattice. The error resulting from this approximation is $O(\delta U^2)$. Clearly the approximation is only good when $\delta U$ is small.

In our simulations we chose $\beta=4.8$. The reason for this value is that we wanted to stay away from the deconfinement transition which one might expect to occur for four flavors somewhere around 5.1.[5] The value of the bare-quark mass was chosen to be 0.1. This may appear large compared to the masses usually used in simulations in the quenched approximation. However, we note that the lattice size considered here is also smaller. Thus, for example, in a Monte Carlo renormalization-group study one would choose $ma=0.04$ on a $16^4$ lattice to compare with the observables obtained here. As we are in the confined region, we expect a good signal for $\bar{\chi}\chi$.

In Fig. 1 we show the plaquette expectation value as a function of the number of iterations for the exact algorithm. It is remarkable that starting from a *completely thermalized quenched* configuration at $\beta=4.8$ the plaquette seems to reach its new value after only a few iterations. This seems to suggest that the effects of dynamical fermions are perhaps rather small. Furthermore, the remarkable flatness of the curve in Fig. 1 leads us to believe that the averages we compute from altogether only 240 iterations are the true averages in the sense that further running would only lead to an improvement in the statistical errors.

At this point we should mention that also the exact algorithm contains a source of error apart from the purely statistical one. In the conjugate-gradient algorithm one calculates the elements of the inverse only to a specified accuracy. We chose to work here with an accuracy per element of the inverse of $\sim2\times10^{-4}$. We believe that this accuracy is sufficient. We do, however, plan to study this question systematically. In the two-dimensional Schwinger model, for example, an accuracy $\delta x_i^2$ of $\sim2\times10^{-3}$ per element seems to be sufficient.[13] Here $\delta x_i^2$ is the square deviation of the $i$th component of $\mathbf{x}$ from the true value when the equation $\mathbf{M}\cdot\mathbf{x}=\mathbf{y}$ is solved for $\mathbf{x}$ by the conjugate-gradient algorithm.

In Table I we have summarized our results for the exact algorithm. The averages shown are obtained by discarding the first fifty iterations. The quoted error in

TABLE II. Summary of our data. (Pseudofermions.)

| $W(1,1)$ | $W(1,2)$ | $W(1,3)$ | $W(2,2)$ | $W(2,3)$ | $W(3,3)$ | $\bar{\chi}\chi/3$ | Acceptance |
|---|---|---|---|---|---|---|---|
| 0.404 | 0.168 | 0.070 | 0.030 | 0.006 | 0.001 | 0.413 | 0.74 |
| (0.002) | (0.002) | (0.001) | (0.001) | (0.001) | (0.001) | (0.009) | |
| 0.416 | 0.180 | 0.078 | 0.037 | 0.008 | 0.001 | 0.409 | 0.86 |
| (0.002) | (0.002) | (0.001) | (0.002) | (0.001) | (0.001) | (0.007) | |

TABLE III. Enhancements of the various expectation values from their quenched values for the exact algorithm and the pseudofermion method at two values of the acceptance.

| $\Delta W(1,1)$ | $\Delta W(1,2)$ | $\Delta W(1,3)$ | $\Delta W(2,2)$ | $\Delta W(2,3)$ | $\Delta W(3,3)$ | $-\Delta(\bar{\chi}\chi)/3$ | Acceptance |
|---|---|---|---|---|---|---|---|
| 0.041 | 0.036 | 0.020 | 0.015 | 0.005 | −0.001 | 0.036 | |
| (0.003) | (0.003) | (0.003) | (0.003) | (0.002) | (0.002) | (0.006) | |
| 0.030 | 0.027 | 0.016 | 0.010 | 0.003 | 0.001 | 0.025 | 0.74 |
| (0.002) | (0.002) | (0.001) | (0.001) | (0.001) | (0.001) | (0.007) | |
| 0.042 | 0.039 | 0.024 | 0.017 | 0.005 | 0.001 | 0.029 | 0.86 |
| (0.002) | (0.002) | (0.001) | (0.001) | (0.001) | (0.001) | (0.008) | |

the plaquette is based on an analysis of the binned fluctuation. This error turns out to be almost identical to the one obtained by considering only every tenth configuration and computing the standard error. The rest of the Wilson loops and $\bar{\chi}\chi$ were, therefore, measured on every tenth configuration. To compute $\bar{\chi}\chi$ we randomly chose ten sites in the lattice and calculated the corresponding thirty diagonal elements of $M^{-1}$ and averaged over them. Table II shows the results of our pseudofermionic simulations at $\beta=4.8$ for two values of the average acceptance: 74% and 86% in the first and second row, respectively. The first value is rather small. Hence one might think that violations of detailed balance are big, although equilibration time is small. We did 2440 iterations in this case, discarding the first 1000 for equilibration. To determine the equilibration time we followed the standard procedure of monitoring various expectation values. Once these are stable apart from fluctuations which are consistent with being purely statistical, we say that equilibrium has been reached. The number of pseudofermionic hits was 24, with four of them discarded. The value of $\bar{\chi}\chi$ was obtained by use of the last 440 iterations. Measurements were made on every twentieth configuration and we did 240 pseudofermion iterations, dropping forty of them to arrive at the value for $\bar{\chi}\chi$ in that configuration. All the errors quoted here have been corrected for correlations from sweep to sweep.[14] In the second case, corresponding to an 86% average acceptance, we essentially repeated the above procedure but with twice as many iterations.

We believe that, considering the rather aggressive choice of parameters in our pseudofermionic calculation, the agreement of the numbers in Tables I and II is remarkably good. This is especially true for the first row of Table II: $\bar{\chi}\chi$ and all the Wilson loops excepting the plaquette and the loop $W(1,2)$ agree within 1 standard deviation, whereas the plaquette and $W(1,2)$ are within 3 standard deviations. One may note, though, that the difference between the two methods appears to be systematic in nature: All Wilson loops are smaller for the pseudofermion method and $\bar{\chi}\chi$ is larger. This is to be expected since at low acceptance in the pseudofermionic method the system will tend to become more disordered. Increasing the acceptance should therefore decrease these systematic differences. Results shown in the second row of Table II are clearly in accord with these naive expectations, as also are those presented in Ref. 9. Results in Table III confirm these expectations even more dramatically. What is shown there is the difference between the expectation values obtained in the theory with dynamical quarks, by the above-mentioned algorithms, and those without them: e.g., $\Delta W(1,1)=W(1,1)_{\text{full}}-W(1,1)_{\text{quenched}}$. Comparing the first row of Table III (exact algorithm) with the second and third (pseudofermion algorithm with 74% and 86% average acceptance), one finds that the agreement between the exact algorithm and the pseudofermions (for the higher acceptance) is remarkable. It shows that the pseudofermion method seems to able to reproduce correctly the effect of fermion loops. We should mention here that we have included $\bar{\chi}\chi$ in Table III for completeness only. $\bar{\chi}\chi$ is a dimensionful quantity and it is therefore not meaningful to compare the quenched and unquenched values. One might argue that good agreement in the quantities we considered only shows that pseudofermions can reproduce the short-distance physics with some accuracy, whereas important physical phenomena such as phase transitions presumably involve fluctuations on all length scales. However, local observables such as the plaquette and $\bar{\chi}\chi$ can be used to monitor, for example, the deconfining and chiral phase transitions. This work shows that there is hope that the pseudofermion method does give the right physics. If this were true, we would be able to make important quantitative predictions about QCD in the presence of dynamical fermions, given present day computing resources.

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