Simulation of $n_f = 3$ QCD by Hybrid Monte Carlo

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Simulations of odd flavors QCD can be performed in the framework of the hybrid Monte Carlo algorithm where the inverse of the fermion matrix is approximated by a polynomial. In this exploratory study we perform three flavors QCD simulations. We make a comparison of the hybrid Monte Carlo algorithm and the R-algorithm which also simulates odd flavors systems but has step-size errors. We find that results from our hybrid Monte Carlo algorithm are in agreement with those from the R-algorithm obtained at very small step-size.

1. Introduction

Recent lattice QCD simulations include effects of dynamical fermions. Due to the algorithmic limitation of the standard Hybrid Monte Carlo (HMC) algorithm \cite{1}, those simulations are limited to even numbers of degenerate flavors. In order to include dynamical effects correctly, simulations of QCD with three flavors (u,d,s quarks) are desirable. Simulations with an odd number of flavors can be performed using the R-algorithm \cite{2}. This algorithm, however, is not exact: it causes systematic errors of order $\Delta \tau^2$, where $\Delta \tau$ is the step-size of the Molecular Dynamics evolution. A careful extrapolation to zero step-size is therefore needed to obtain exact results. Nevertheless, it is common practice to forego this extrapolation and to perform simulations with a single step-size chosen small enough that the expected systematic errors are smaller than the statistical ones. We want to point out that there is an alternative to the R-algorithm, which gives arbitrarily accurate results without any extrapolation\cite{3}.

Lüscher proposed a local algorithm, the so-called "Multiboson algorithm" \cite{4}, in which the inverse of the fermion matrix is approximated by a suitable Chebyshev polynomial. Originally he proposed it for two flavors QCD. Borici and de Forcrand \cite{5} noticed that the determinant of a fermion matrix can be written in a manifestly positive way using a polynomial approximation, so that one can simulate odd flavors QCD with the multiboson method. Indeed, using this method, one flavor QCD was simulated successfully \cite{6}. The same polynomial approximation can be applied for the HMC \cite{7}. Actually, in the development stage of Ref.\cite{7}, one flavor QCD was also simulated by HMC and it was confirmed that the two algorithmically different methods — multiboson and HMC — give the same plaquette value \cite{6}. Here we give the formulation of the HMC algorithm with odd flavors and perform $n_f = 3$ QCD simulations. Then we compare our results with those of the R-algorithm.

2. Formulation

2.1. $n_f = 2$

The application of Lüscher’s idea \cite{4} to $n_f = 2$ QCD HMC was first made by the authors of Ref.\cite{7}, and later by \cite{8}. The lattice QCD partition function with $n_f = 2$ degenerate quark flavors is given by

$$Z = \int dU \det D^2 \exp(-S_{\text{gauge}}), \quad (1)$$

where $D$ is the fermion matrix and in this study we use Wilson fermions. In the formulation of the
HMC algorithm, \( \det D^2 \) is treated as

\[
\det D^2 \sim \int d\phi d\phi^{\dagger} \exp(-\phi^{\dagger} D^{\dagger -1} D^{-1} \phi),
\]

(2)

where the \( \gamma_5 \) hermiticity of the fermion matrix \( D \), i.e. \( D = \gamma_5 D^{\dagger} \gamma_5 \), is used.

Introducing momenta \( P \) conjugate to the link variables \( U \), the partition function is rewritten as

\[
Z = \int dU dP \exp(-H),
\]

(3)

where the Hamiltonian \( H \) is defined by

\[
H = \frac{1}{2} P^2 + S_{\text{gauge}} + \phi^{\dagger} D^{\dagger -1} D^{-1} \phi.
\]

(4)

This Hamiltonian is used for the Molecular Dynamics (MD) simulation of the standard HMC algorithm. Eq. (4) has a computational difficulty in the Multiboson algorithm. Our algorithm will tend to reject these configurations at the Metropolis step, leading to extremely long autocorrelation times. This domain of convergence can be changed by adopting another approximating polynomial. However, the origin must be excluded. Together with connectness and conjugate symmetry of the spectrum, this implies that the real negative axis is always excluded from the domain of convergence for any polynomial. Configurations with real negative Dirac eigenvalues will be rejected by our polynomial algorithm.

2.2. \( n_f = 1 \)

After invention of the multiboson algorithm, Borici and de Forcrand noticed that a single \( \det D \) can be treated in a manifestly positive way and an \( n_f = 1 \) multiboson simulation was performed to study thermodynamics of \( n_f = 1 \) QCD.

As before, the inverse of the fermion matrix \( D \), using a polynomial of degree \( 2n \), is approximated as

\[
1/D \approx \prod_{k=1}^{2n} (D - Z_k),
\]

(7)

where \( Z_k = 1 - \exp(i 2\pi k/(2n + 1)) \). Noticing that the \( Z_k \)'s come in complex conjugate pairs, eq. (7) is rewritten as

\[
1/D \approx \prod_{k=1}^{n} (D - \bar{Z}_k)(D - Z_k).
\]

(8)

Using the \( \gamma_5 \) hermiticity of the fermion matrix, we find that \( \det(D - \bar{Z}_k) = \det(D - Z_k)^\dagger \). Thus the determinant of \( D \) is written as

\[
\det(D) \sim \det(T_n^\dagger(D)T_n(D))^{-1},
\]

(9)

where \( T_n(D) \equiv \prod_{k=1}^{n}(D - Z_k) \), and then we obtain

\[
\det(D) \sim \int d\phi d\phi^{\dagger} \exp(-\phi^{\dagger} T_n^\dagger(D)T_n(D)\phi).
\]

(10)

The term \( \phi^{\dagger} T_n^\dagger(D)T_n(D)\phi \) is manifestly positive. Then we may define the Hamiltonian of \( n_f = 1 \)
QCD as
\[ H = \frac{1}{2} P^2 + S_{\text{gauge}} + \phi^i T_n(D) T_n(D) \phi. \] (11)
With this Hamiltonian there is no difficulty to perform HMC algorithm. To improve efficiency and accuracy, one may use a polynomial of lower degree \( n \) during the Molecular Dynamics trajectory, and a much higher degree \( m \gg n \) for the Metropolis step \cite{10}. The domain of convergence of the approximation eq.(10) is the same as for \( n_f = 2 \). Exceptional configurations for which eigenvalues fall outside this domain will likewise be rejected at the Metropolis step. A further difficulty is that the sampled measure is \( \propto \operatorname{det}(T_n(D) T_n(D))^{-1} \), which for exceptional configurations differs from the desired \( \operatorname{det} D \), increasingly so with \( n \).

2.3. \( n_f = 2 + 1 \)
The partition function of \( n_f = 2 + 1 \) QCD is given by
\[ Z = \int dU \operatorname{det} \tilde{D}^2 \operatorname{det} D \exp(-S_{\text{gauge}}), \] (12)
where the notations \( \tilde{D} \) and \( D \) are introduced to distinguish the two different quark masses. Using eq.(2) for \( \operatorname{det} \tilde{D} \) and eq.(10) for \( \operatorname{det} D \),
\[ \operatorname{det} \tilde{D}^2 \operatorname{det} D \sim \int d\tilde{\phi}^i d\phi^i d\phi \exp(\tilde{\phi}^i \tilde{D}^i - \phi^j D^j - H_T), \] (13)
where \( H_T \equiv \phi^i T_n(D) T_n(D) \phi \). We define \( n_f = 2 + 1 \) Hamiltonian by
\[ H = \frac{1}{2} P^2 + S_g + \tilde{\phi}^i \tilde{D}^i - \phi^j D^j + H_T. \] (14)
Two remarks are in order: (i) as for \( n_f = 1 \), one could use during the MD trajectory a polynomial of lower degree than for the Metropolis step; (ii) the two bosonic fields \( \phi \) and \( \tilde{\phi} \) could be replaced by a single one, with action \( \phi^i T_n(D) \tilde{D}^i - \phi^j D^j T_n(D) \phi \). For simplicity, in this exploratory study we use two distinct bosonic fields and a single approximating polynomial.

3. Convergence
3.1. \( n_f = 2 \)
To see the rate of convergence of \( P_n(D) \), we calculate the quantity \( X_n = \phi^i P_n(D) P_n(D) \phi \).

In the limit \( n \to \infty \), \( X_n \) goes to \( X_{\text{exact}} \equiv \phi^i \tilde{D}^i - \phi^j D^j \). First, we choose \( X_{\text{exact}} = \eta^i \eta \) where \( \eta \) is a random gaussian vector. Then the vector \( \phi \) is set to \( \phi = D \eta \). The accuracy of \( X_n \) is measured by the difference between \( X_n \) and \( X_{\text{exact}} \). We use a random gauge configuration. Figure 1:(top) shows \( X_n \) versus the degree \( n \) for different quark masses. Here the same \( \eta \) is used for each calculation of \( X_n \). \( X_n \) converges to one value as \( n \) increases, but at high degree \( n \), \( X_n \) diverges, which can be understood due to the rounding errors of our computer, where calculations are performed with 64-bit accuracy. Figure 1:(bottom) shows the accuracy of \( X_n \) by \( |X_n - X_{\text{exact}}| \). Exponential convergence is seen for each quark mass, but the rate of convergence is slow for small quark masses.
3.2. $n_f = 1$

We do the same analysis as for $n_f = 2$, but for $n_f = 1$, the value of $X_{\text{exact}}$ is not known. So we calculate the quantity $X_n = \phi^\dagger T_n(D) T_n(D) \phi$, where the vector $\phi$ is a gaussian random vector, and we use a random gauge configuration. We assume that $X_n$ goes to a certain value in the limit of $n \to \infty$. Figure 2:(top) shows $X_n$ as a function of degree $n$. $X_n$ seems to converges to a certain value when the degree $n$ increases. At high degree $n$, $X_n$ diverges as in the case of $n_f = 2$.

To see the rate of convergence, we calculate $|X_n - X_{\text{max}}|$ where $X_{\text{max}}$ is defined by $X_{\text{max}} = X_m$, $m \gg n$. Due to the rounding errors, we can not take $m$ very large. We take a maximum number $m$ where the rounding errors still do not appear. Figure 2:(bottom) shows $|X_n - X_{\text{max}}|$ as a function of degree $n$. The dips seen in the figure are just due to the fact that at those points $X_n = X_{\text{max}} = X_m$. The convergence seems to be exponential, but the rate of convergence is slow for small quark masses as in the $n_f = 2$ case.

4. Simulations

Simulations of three flavors QCD are performed on an $8^2 \times 10 \times 4$ lattice at $\beta = 5.0$ with $\kappa = 0.130$ and 0.160. We measure the plaquette and Polyakov loop varying the degree $n$ and compare them with those from the R-algorithm obtained.
with a step-size $\Delta \tau = 0.01$. Figures 3 and 4:(top) show the plaquette as a function of $n$ at $\kappa = 0.130$ and $0.160$, respectively. Except for very small $n$, the results from the HMC algorithm agree with those from the R-algorithm within statistical errors. Results of the Polyakov loop are shown in Figures 3 and 4:(bottom). Except for a small discrepancy seen in Figure 3, the results from the HMC algorithm are in agreement with those from the R-algorithm. Note that convergence is not monotonic in $n$.

5. Conclusions

We formulated an odd-flavor HMC algorithm using a polynomial approximation. Simulations of three flavors QCD were performed. We found that the plaquette values are consistent with those from the R-algorithm at very small step-size. In principle the HMC algorithm is able to simulate any flavors of QCD, with arbitrary accuracy and without extrapolation [as long as all Dirac eigenvalues are not real negative]. However the rounding errors should be under control when we use a large lattice or/and small quark masses where one may need a polynomial of high degree $n$ to achieve sufficient approximation.

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