An exact algorithm for three-flavor QCD with $O(a)$-improved Wilson fermions *

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We present an exact dynamical QCD simulation algorithm for the $O(a)$-improved Wilson fermion with odd number of flavors. Our algorithm is an extension of the non-Hermitian polynomials HMC algorithm proposed by Takaishi and de Forcrand previously. In our algorithm, the systematic errors caused by the polynomial approximation of the inverse of Dirac operator is removed by a noisy-Metropolis test. For one flavor quark it is achieved by taking the square root of the correction matrix explicitly. We test our algorithm for the case of $N_f = 1 + 1$ on a moderately large lattice size ($16^3 \times 48$). The $N_f = 2 + 1$ case is also investigated.

1. Introduction

Lattice QCD simulations with three flavors of dynamical quarks are indispensable to understand the low energy QCD dynamics in the real world. Takaishi and de Forcrand [1] have proposed a Hybrid Monte Carlo (HMC) algorithm which can treat odd number of flavors of dynamical quarks, in which a non-Hermitian polynomial approximation is applied to the inverse of the Wilson-Dirac operator. Very recently they have removed the systematic error from the polynomial approximation, making their algorithm exact [2].

For realistic simulations with the available computational power, the $O(a)$-improvement program is widely advocated. We then extend the algorithm of Refs. [1,2] to the $O(a)$-improved Wilson quark actions. We also develop a noisy-Metropolis test to remove the systematic error from the polynomial approximation, which is different from that of Ref. [2].

In this article, we describe our algorithm for single flavor of dynamical quark. The consistency with the usual algorithm and applicability to large-scale simulations are examined by running the N_f=1+1 and N_f=2 simulations on a $16^3\times48$ lattice. Employing the algorithm, we have started a search for the lattice parameters (β, κ etc.) suitable for realistic simulations with N_f=2+1 flavors of quarks (*i.e.,* degenerate up-down quarks and strange quark). We briefly describe the novel findings from the search, referring to a separate report [5] for details.

*Presented by K-I. Ishikawa

2. Algorithm

Our HMC algorithm for single flavor of dynamical quark is based on the following QCD partition function:

$$\mathcal{Z} = \int \mathcal{D}[U] \det[(1+T)] \det[\hat{D}_{oo}] e^{-S_{\rm g}[U]}, \qquad (1)$$

where $S_{\rm g}[U]$ is the plaquette gauge action and $\hat{D}_{oo}$ is the symmetrically preconditioned $O(a)$-improved Wilson-Dirac operator defined by

$$\hat{D}_{oo} = 1 - (1+T)^{-1}_{oo} M_{oe} (1+T)^{-1}_{ee} M_{eo}, \qquad (2)$$

where the subscript e (o) means the even (odd) components of the Dirac operator. The factor T is the local SW-term of the $O(a)$-improved Wilson-Dirac operator and M is the hopping matrix. There is another even-odd preconditioning in which only the even-even (or odd-odd) SW-term is asymmetrically factored out. We compared the efficiency of the symmetric and asymmetric preconditionings within the usual N_f=2 HMC algorithm, and found that the former has better efficiency. Therefore we employ the symmetrically preconditioned form for the QCD partition function. (For other preconditioning techniques, see Ref. [3].)

Using the trick described in Refs. [1,2,4], we rewrite the determinant of the Dirac operator as

$$\det[\hat{D}_{oo}] = \frac{\det[\hat{D}_{oo} P_{N_{poly}}[\hat{D}_{oo}]]}{\det[P_{N_{poly}}[\hat{D}_{oo}]]} = \frac{\det[W_{oo}]}{|\det[T_{N_{poly}}[\hat{D}_{oo}]]|^2}, \quad (3)$$

where $P_{N_{poly}}[z]$ is a non-Hermitian polynomial of order N_{poly} (assumed to be even) defined by $P_{N_{poly}}[z]=\sum_{i=0}^{N_{poly}} c_i (z-1)^i$ which approximates $1/z$, and $W_{oo} \equiv \hat{D}_{oo} P_{N_{poly}}[\hat{D}_{oo}]$. $T_{N_{poly}}[z]$ is a kind of square root of $P_{N_{poly}}[z]$ defined by $P_{N_{poly}}[z] = T^*_{N_{poly}}[z] T_{N_{poly}}[z]$ with $T_{N_{poly}}[z]=\sum_{i=0}^{N_{poly}/2} d_i (z-1)^i$. We employ the Chebyshev polynomial approximation (*i.e.,* the hopping matrix expansion) for $P_{N_{poly}}[z]$ and hence the coefficients are $c_i=(-1)^i$. We use the Clenshaw's recurrence formula to calculate these polynomials.

Introducing pseudo fermion fields ψ_o for $|\det[T_{N_{poly}}[\hat{D}_{oo}]]|^2$ in Eq. (3), Eq. (1) becomes

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}[U,\psi_o] \det[W_{oo}] e^{-S_{eff}[U,\psi_o]}, \\ S_{eff}[U,\psi_o] &= S_{\rm g}[U] + S_{\rm det}[U] + S_{\rm q}[U,\psi_o], \\ S_{\rm det}[U] &= -\log[\det[(1+T)]], \\ S_{\rm q}[U,\psi_o] &= |T_{N_{poly}}[\hat{D}_{oo}]\psi_o|^2. \end{aligned} \quad (4)$$

Our PHMC algorithm consists of the following two steps in this case: 1) the usual HMC algorithm for the effective action S_{eff}, 2) the noisy-Metropolis test for the correction term $\det[W_{oo}]$. The noisy-Metropolis test is carried out only after accepting the HMC Metropolis test.

The acceptance probability of the noisy-Metropolis test is defined by

$$P_{corr}[U \to U'] = \min[1, e^{-dS}],$$

$$dS = |A_{oo}[U']^{-1} A_{oo}[U] \chi_o|^2 - |\chi_o|^2, \quad (5)$$

where U is an initial configuration and U' is a trial configuration generated by the preceding HMC algorithm. Here χ_o is a random vector with Gaussian distribution, and A_{oo} is defined by $A_{oo}^2 = W_{oo}$. This algorithm estimates $|\det[A_{oo}]|^2$ instead of $\det[W_{oo}]$. A_{oo} and A_{oo}^{-1} are evaluated by the Taylor expansion with respect to $W_{oo}-1$. In order to keep the exactness of our algorithm the residual of the Taylor expansion is monitored whenever Eq. (5) is calculated. Our programs are written in double precision arithmetic, and optimized for HITACHI SR8000 at KEK.

3. $N_f = 1+1$

We test our single-flavor algorithm by additively combining two single-flavored pseudo fermions (N_f=1+1) and comparing results with those of the usual N_f=2 HMC algorithm. In this case our algorithm runs as follows: 1) the HMC algorithm with the two single-flavored pseudo fermions, 2) the noisy-Metropolis test for each correction terms, which is carried out only when the preceding Metropolis test is accepted. To check viability of our algorithm toward realistic simulations, we employ a moderately large-scale simulation parameter: $16^3 \times 48$, β=5.2, $c_{\rm SW}$=2.02, κ=0.1340 and κ=0.1350. These hopping parameters correspond to $m_\pi/m_\rho \sim 0.8$ and ~ 0.7, respectively.

Figure 1 shows the convergence of $T_{N_{poly}}[\hat{D}_{oo}]$ as N_{poly} increases. The measurement is made on 20 configurations separated by 10 trajectories. The residual is defined by $|T^*_{N_{poly}}[\hat{D}_{oo}] T_{N_{poly}}[\hat{D}_{oo}] \hat{D}_{oo} \eta_o - \eta_o| / |\eta_o|$ with a Gaussian noise vector η_o. We observe an exponential decay as expected and there are no accumulation of round-off errors for large N_{poly}.

We also investigate the reversibility of the molecular dynamics step and observe that the violation stays around the limit of double precision for both of the quark masses (see Fig. 2 for κ= 0.1350). The value of plaquette, averaged over $\sim$1000 trajectories, is consistent between the two algorithms (*e.g.*, $\langle P \rangle$=0.53393(11)(HMC) and 0.53392(9)(PHMC with N_{poly}=140) for κ=0.1350). With these observation we conclude

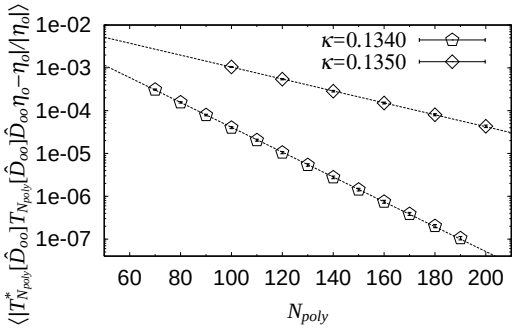

Figure 1. Convergence $T_{N_{poly}}[\hat{D}_{oo}]$ as $N_{poly} \to \infty$.

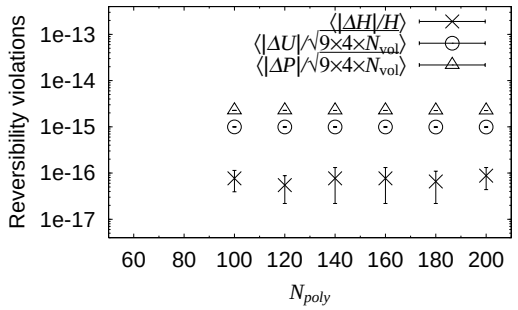

Figure 2. N_{poly} dependence of the reversibility violations at $\kappa = 0.1350$. $|\Delta H|/H$: total Hamiltonian, ΔU: gauge link, ΔP: gauge momentum.

that our PHMC algorithm for single-flavor dynamical quark works well on moderately large lattices and intermediate quark mass for at least N_f=1+1.

4. $N_f = 2 + 1$

For the N_f=2+1 case, we additively combine the standard two-flavored pseudo fermion and our single-flavored pseudo fermion as suggested in Refs. [1,2]. The algorithm is given by 1) the HMC step with the combined effective Hamiltonian, and 2) the noisy-Metropolis test for the correction factor.

We compare results for the averaged plaquette between our algorithm and the Hybrid-R algorithm on a $4^3\times8$ lattice at β=4.8, $c_{\rm SW}$=1.0, κ_{ud}=0.150, and κ_s=0.140. Figure 3 shows the molecular dynamics step size dt dependence of the plaquette value with the Hybrid-R and PHMC(N_{poly}=10) algorithms. The results with the PHMC algorithm (squares) do not depend on dt and are consistent with the

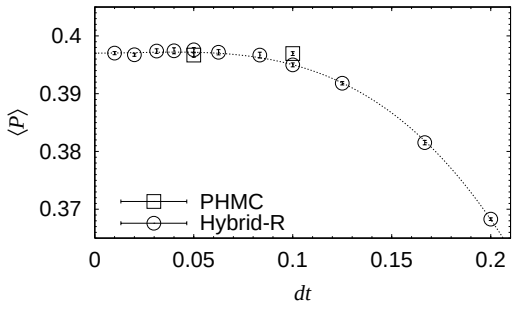

Figure 3. Plaquette vs dt.

value at $dt \to 0$ with the Hybrid-R algorithm ($\langle P\rangle$=0.39669(38)(PHMC), 0.39702(12)(Hybrid-R)).

Encouraged with these results, we haved performed a series of parameter searches that would realize a^{-1}∼1–2 GeV, L∼1–2 fm, m_π/m_ρ∼0.7–0.8 on a $12^3\times32$ lattice. During the search, which employed the tadpole-improved one-loop value for $c_{\rm SW}$ and degenerate quark mass (N_f=3), we have found an unexpected first-order phase transition around β∼4.8–5.0 . This phase transition is also observed with the Hybrid-R algorithm on a $8^3\times16$ lattice with the same lattice parameter. The details of the phase structure are given in Ref. [5].

This work is supported by the Supercomputer Project No.66 (FY2001) of High Energy Accelerator Research Organization (KEK), and also in part by the Grant-in-Aid of the Ministry of Education (Nos. 10640246, 11640294, 12014202, 12640253, 12640279, 12740133, 13640260 and 13740169). K-I.I. and N.Y. are supported by the JSPS Research Fellowship.

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