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Non-trivial phase structure of $N_f = 3$ QCD with $O(a)$-improved Wilson fermion at zero temperature *

JLQCD Collaboration: S. Aoki[a], R. Burkhalter[a,b], M. Fukugita[c], S. Hashimoto[d], K-I. Ishikawa[d], N. Ishizuka[a,b], Y. Iwasaki[a,b], K. Kanaya[a,b], T. Kaneko[d], Y. Kuramashi[d], M. Okawa[d], T. Onogi[e], S. Tominaga[b], N. Tsutsui[d], A. Ukawa[a,b], N. Yamada[d], T. Yoshié[a,b]

[a]Institute of Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan

[b]Center for Computational Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8577, Japan

[c]Institute for Cosmic Ray Research, University of Tokyo, Kashiwa, Chiba 277-8582, Japan

[d]High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305-0801, Japan

[e]Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan

JLQCD collaboration recently started the $N_f = 3$ QCD simulations with the $O(a)$-improved Wilson fermion action employing an exact fermion algorithm developed for odd number of quark flavors. It is found that this theory has an unexpected non-trivial phase structure in the (β, κ) plane even at zero temperature. A detailed study is made to understand the nature of the observed phase transitions and to find the way of avoiding untolerably large lattice artifacts associated with the phase transition.

1. Introduction

Including the dynamical quark loop effects in large-scale QCD simulations is one of the most important and urgent problem. While in the real world there are three light quarks, most of recent studies have concentrated on the case of two flavors of Wilson-type fermions because these systems can be simulated by the exact Hybrid Monte Carlo (HMC) algorithm. Recently, however, a major progress has been made in the exact fermion algorithm applicable to odd number of flavors as reviewed in Ref. [1]. In particular, we have succeeded in developing an efficient algorithm for $N_f = 3$ QCD with the $O(a)$-improved Wilson fermion action in the framework of the HMC algorithm. Leaving algorithmic details to a separate report [2], we present here the first result toward realistic $N_f = 3$ QCD simulations with the $O(a)$-improved Wilson fermion. We found that this theory has an unexpected first-order phase transition at zero-temperature, which gives a strong constraint on the form of lattice actions suitable for large-scale simulations.

*Presented by M. Okawa.

2. Phase structure for plaquette gauge action

The partition function we study is defined by

$$\mathcal{Z} = \int \mathcal{D}U \, (\det[D_{ud}])^2 (\det[D_s]) e^{-S_g(U)}. \tag{1}$$

Here $S_g(U)$ is the gluon action

$$S_g(U) = \frac{\beta}{6}\left[c_0 \sum W_{1\times1} + c_1 \sum W_{1\times2}\right], \tag{2}$$

where $c_0 = 1 - 8c_1$ and $W_{1\times1}$ and $W_{1\times2}$ are the plaquette and rectangular Wilson loops, respectively, and $(\det[D_{ud}])^2$ represents the contribution from degenerate u and d quarks whereas s quark effect is given by $(\det[D_s])$ with $D_q(q = ud, s)$ the $O(a)$-improved Wilson-Dirac operator.

We start our analysis employing the plaquette gauge action ($c_1 = 0$), determining the clover coefficient $c_{\rm sw}$ by tadpole-improved one-loop perturbation theory;

$$c_{\rm sw} = \frac{1}{\langle P\rangle^{\frac{3}{4}}}\left(1 + 0.0159\frac{6/\beta}{\langle P\rangle}\right), \tag{3}$$

with $\langle P\rangle$ evaluated in the quenched approximation at the corresponding value of β.

Given the lattice action, we have three tunable parameters, the gauge coupling β, the hopping

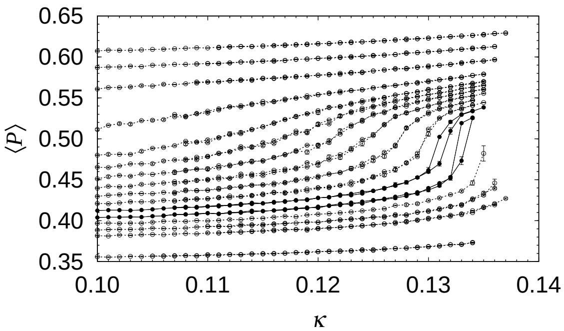

Figure 1. Thermal cycles on an $8^3 \times 16$ lattice at $\beta = 4.6$, 4.8, 4.85, 4.9, 4.95, 5.0, 5.05, 5.1, 5.15, 5.2, 5.25, 5.3, 5.4, 5.6, 5.8, 6.0 from bottom to top.

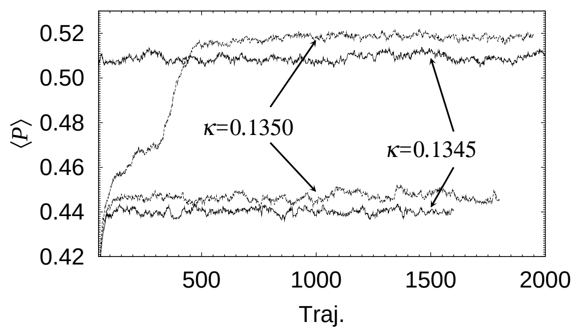

Figure 2. Two-state signals on a $12^3 \times 32$ lattice at β=4.88 and $c_{\rm sw}$=2.15.

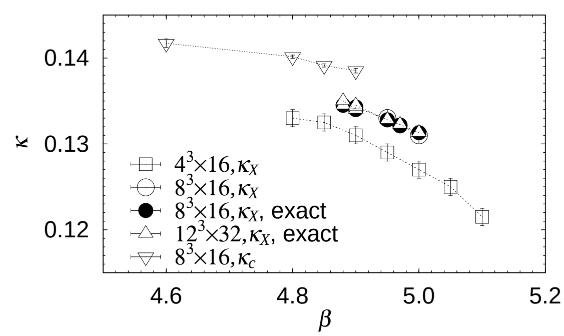

Figure 3. Phase diagram in (β, κ) plane.

parameter κ_{ud} for ud quarks and κ_s for s quark. For simplicity we set $\kappa_{ud} = \kappa_s \equiv \kappa$ in this work. To see the global phase structure in the (β, κ) plane, we perform rapid thermal cycles on $4^3 \times 16$ and $8^3 \times 16$ lattices. Fixing β we increase κ from $\kappa = 0$ in steps of 0.01 until the algorithm fails to converge and then decrease κ to 0. The procedure is repeated for several values of β. In this analysis, we omit the noisy Metropolis test for the correction factor $\det[W_{oo}]$ [2] and fix the order of the Chebyshev polynomial to $n = 100$.

The result of the thermal cycle on an $8^3 \times 16$ lattice is shown in Fig. 1. We clearly observe hysteresis loops at $\beta = 4.95$ and 5.0. On a $4^3 \times 16$ lattice, the hysteresis loop is seen in a wider range of β at $4.8 \leq \beta \leq 5.1$. To understand the nature of the hysteresis in more detail, we perform simulations starting from both ordered and disorder configurations with fixed values of β and κ on $8^3 \times 16$ and $12^3 \times 32$ lattices. Some examples are shown in Fig. 2. Here we make simulations exact by including the correction factor $\det[W_{oo}]$. We observe clear two state signals for several sets of parameters, which demonstrates that the hysteresis in the thermal cycles is caused by a first-order phase transition.

In Fig. 3 we plot the location of the observed phase transition line ($\kappa = \kappa_X(\beta)$) on the (β, κ) plane for $8^3 \times 16$(filled circles) and $12^3 \times 32$ (open upper-triangles) lattices. Also shown in Fig. 3 are the location of the hysteresis observed on $4^3 \times 16$ and $8^3 \times 16$ lattices (open squares and circles). The position of the phase transition line significantly moves from $4^3 \times 16$ to $8^3 \times 16$. However, it stays in the same place when the lattice size increases from $8^3 \times 16$ to $12^3 \times 32$. In Fig. 4, we plot the plaquette values in the two phases at the phase transition line as functions of β for $8^3 \times 16$ and $12^3 \times 32$ lattices. The gap in the plaquette is almost independent of the lattice size. These findings strongly suggests that the first-order transition line persists in infinite lattice volume and zero temperature.

Figure 4 also shows that the gap in the plaquette decreases almost linearly in β and vanishes at around $\beta = 5.0$. Since no signs of transitions are observed at $\beta > 5.0$ in Fig. 1, we do not think that this point corresponds to a tricritical point where a first-order phase transition line changes to a second-order one which then extends toward weaker couplings. Rather, the observed first-order transition must be a lattice artifact restricted to strong coupling regions.

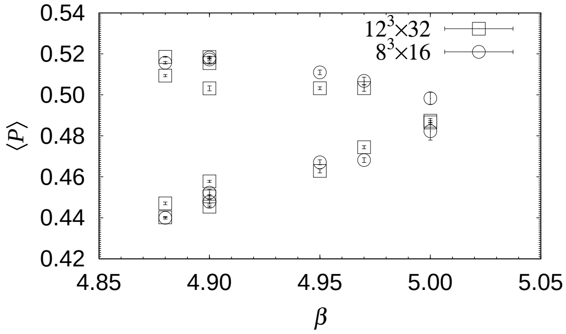

Figure 4. Plaquette values in two phases at the first-order transition line as functions of β.

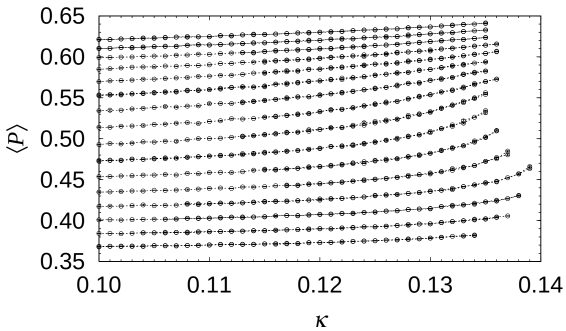

Figure 5. Thermal cycle with RG gauge action at β=1.50−2.25 in steps of 0.05 (bottom to top).

3. Phase structure for improved gauge action

To confirm this possibility, we repeat thermal cycle simulations employing the improved gauge action with $c_1 = -0.331$ (RG action [3]) and $c_1 = -1/(12\langle P\rangle^{\frac{1}{2}})$ (tadpole-improved Symanzik action [4]). Here $c_{\rm sw}$ is again determined by tadpole-improved one-loop perturbation theory. Figure 5 shows the result of thermal cycles for the RG action on an $8^3 \times 16$ lattice. No signs of hysteresis loops are seen, and hence non-trivial phase structure is absent with this gauge action. Hysteresis is also not seen for the tadpole-improved Symanzik gauge action. We conclude that the first-order phase transition observed for the plaquette gauge action has the nature of a lattice artifact.

4. Implications

It has been known [5] that pure $SU(3)$ gauge theory with fundamental and adjoint couplings has a first-order transition for positive values of the adjoint coupling. It is an interesting possibility that the clover term produces a positive adjoint coupling in an effective theory after integrating out the fermion degrees of freedom, which eventually causes the first-order phase transition observed in this work. In fact we have checked that there are no sign of phase transitions in thermal cycles made with the unimproved Wilson fermion action ($c_{\rm sw} = 0$) and plaquette gauge action ($c_1 = 0$) on a $8^3 \times 16$ lattice, which supports our interpretation.

Our finding poses a serious practical problem whether realistic simulations with reasonable values of the lattice spacing a are possible with the $O(a)$-improved Wilson fermion and the plaquette gauge action. To study this problem, we evaluate the lattice spacing from static quark potential at $\beta = 5.0$. Our results are $a^{-1} = 1.53(2)$ GeV ($\kappa = 0.1320$), 2.06(5) GeV ($\kappa = 0.1330$) and 2.58(4) GeV ($\kappa = 0.1338$). Continuum extrapolations using lattices with a^{-1} starting at 2.58 GeV is not practical. Our natural choice, then, is to use improved gauge actions for realistic $N_f = 3$ QCD simulations with the $O(a)$-improved Wilson fermion.

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