Exploring QCD at small sea quark masses with improved Wilson-type quarks*

CP-PACS Collaboration : Y. Namekawa[a], S. Aoki[a], M. Fukugita[b], K-I. Ishikawa[a,c], N. Ishizuka[a,c], Y. Iwasaki[a], K. Kanaya[a], T. Kaneko[d], Y. Kuramashi[d], V.I. Lesk[c], M. Okawa[e], Y. Taniguchi[a], A. Ukawa[a,c], T. Umeda[c], and T. Yoshié[a,c]

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

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

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

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

[e]Department of Physics, Hiroshima University, Higashi-Hiroshima 739-8526, Japan

We explore the region of small sea quark masses below $m_{PS}/m_V = 0.5$ in two-flavor QCD using a mean-field improved clover quark action and an RG-improved gauge action at $a \simeq 0.2$ fm on $12^3 \times 24$ and $16^3 \times 24$ lattices. We find that instability of the standard BiCGStab algorithm at small quark masses can be mostly removed by the BiCGStab(DS-L) algorithm, which employs L-th minimal residual polynomials with a dynamical selection of L. We also find singular spikes of ΔH in the HMC algorithm at moderate values of $\Delta\tau$. Nature of the spike is studied. We also study finite-size effects and chiral properties of meson masses.

1. Introduction

A rapid increase of the computational cost and instabilities in simulation algorithms have so far limited simulations of QCD with dynamical Wilson-type quarks to quark masses corresponding to $m_{PS}/m_V \gtrsim 0.6$ [1], to be compared with the physical value $m_\pi/m_\rho = 0.18$. This limitation of the range of quark masses causes sizable ambiguities and systematic errors in the extrapolation to the physical point. A related problem is that the mass dependences predicted by chiral perturbation theory (ChPT) have not been confirmed in full QCD simulations [1–3].

In this report, we explore the light quark mass region extending our previous systematic study of two-flavor QCD [4]. Through an improvement of simulation algorithms, sea quark masses corresponding to $m_{PS}/m_V = 0.6$–0.4 are studied on coarse lattices with $a \simeq 0.2$ fm.

We adopt a renormalization-group improved gauge action and a meanfield-improved clover quark action [4]. At $\beta = 1.8$ ($a \simeq 0.2$fm), we employ $12^3 \times 24$ and $16^3 \times 24$ lattices with the spatial size 2.4 and 3.2 fm. Simulation parameters and present statistics are summarized in Table 1. Measurements are done at every 5 trajectories generated by the HMC algorithm.

2. Inversion of the quark matrix

In Ref. [4], the BiCGStab algorithm is adopted to invert the quark matrix. At small quark masses, the BiCGStab sometimes fails to converge. While the CG algorithm is guaranteed to converge, it is quite time-consuming. We find that an extension of BiCGStab to L-th order minimal residual polynomials, the BiCGStab(L) algorithm [5], is more stable. The conventional BiCGStab corresponds to the case $L = 1$.

A larger L is expected to lead to a better convergence. In practice, however, too large L is time-consuming and also frequently introduces other instabilities. Figure 1 shows the L-dependence of the residual on a test configura-

*Talk presented by Y. Namekawa

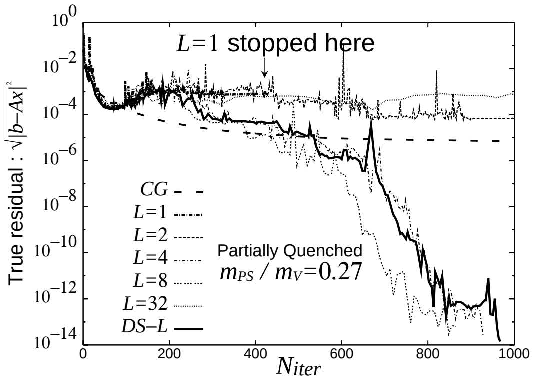

Figure 1. True residual at $(m_{PS}/m_V)_{val} = 0.27$ as a function of L and N_{iter} measured on a configuration at $(m_{PS}/m_V)_{sea} = 0.6$.

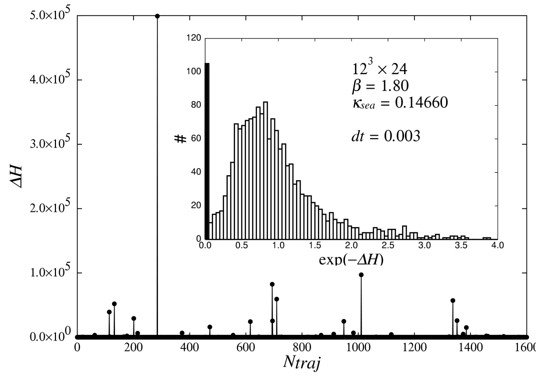

Figure 2. Time history of ΔH and the corresponding histogram of $\exp(-\Delta H)$.

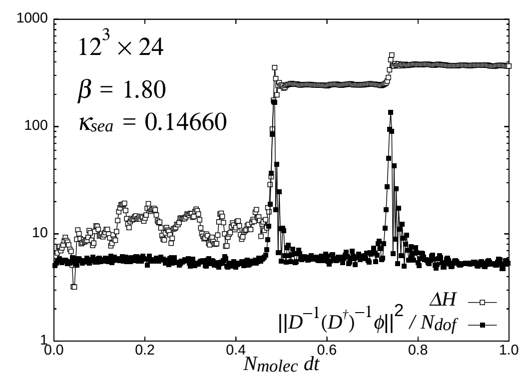

Figure 3. ΔH and the quark force at a spike.

tion. Optimum values of L depend on the simulation parameters.

To avoid a tuning of L at each simulation point, we employ the BiCGStab(DS-L) algorithm [6]. This is an improvement of BiCGStab(L) in which an optimum L is dynamically selected. We find that BiCGStab(DS-L) is much more robust than the original BiCGStab at small quark masses without much increase of the computer time.

3. HMC updates

Another difficulty at small quark masses is the appearance of instabilities in MD evolutions of the HMC algorithm. Figure 2 is an example of the time history of $\Delta H \equiv H_{trial} - H_{old}$ at $m_{PS}/m_V = 0.5$. We observe that ΔH sometimes shows huge values ("spikes"). A similar phenomenon has been reported in [7]. A consequence of the spikes is a distorted distribution of $e^{-\Delta H}$ at $e^{-\Delta H} \approx 0$ (see the inset of Fig. 2). While the trial configurations with large ΔH are automatically rejected by the HMC algorithm, the distortion of the $e^{-\Delta H}$ distribution can introduce additional systematic errors (within the statistical errors) through the accept/reject process.

We find that the frequency of spikes decreases as we decrease the MD step size dt. We have also checked that spikes do not violate the reversibility and area-preservation required by the HMC algorithm.

In order to clarify the origin of spikes, we plot $\Delta H(p(t), U(t+\frac{1}{2}dt))$ and $||D^{-1}(D^{\dagger})^{-1}\phi||$ for the quark force as functions of the MD time t on a configuration with a spike, where p is the conjugate momentum of U and ϕ is the pseudo-fermion field. From Fig. 3, we find that ΔH jumps to a large value when the quark force becomes large. We confirm that the quark force remains small when dt is small enough to remove spikes.

A mechanism to induce large ΔH from large

Table 1
Simulation parameters and number of trajectories at $\beta = 1.8$.

$(m_{PS}/m_V)_{sea}$		0.6	0.5	0.4
κ_{sea}		0.14585	0.14660	0.14705
N_{traj}	$12^3 \times 24$	3500	3500	2100
	$16^3 \times 24$	1400	750	–

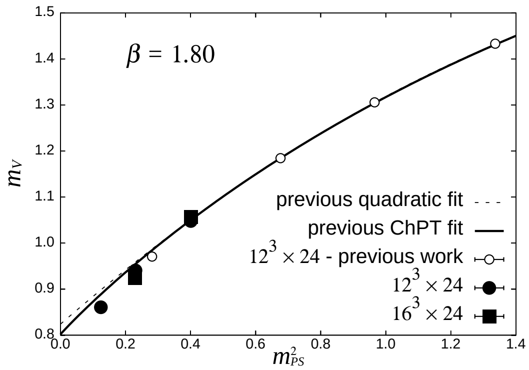

Figure 4. Pseudo-scalar and vector meson masses.

force is described in [8]. In a simple harmonic oscillator system with the frequency ω, a discrete approximation of the MD evolution becomes unstable for $dt > 2/\omega$ and ΔH diverges exponentially with the MD time. This suggests that the discretized MD evolution of HMC with fixed dt may become unstable if an effective $\omega \propto \sqrt{\text{force}}$ in QCD exceeds a critical value. To study the origin of large force, we are currently investigating the eigenvalues of the quark matrix.

4. Meson masses

Our preliminary results for the pseudo-scalar and vector meson masses are shown in Fig. 4, together with the previous results at the same β [4]. We note that the new data points are consistent with the previous data in the overlapping region, but show a deviation from the chiral extrapolation fit curves of the previous data, at small quark masses. The difference amounts to 3% (2.5σ) in the chiral limit. Comparing the results from $12^3 \times 24$ and $16^3 \times 24$ lattices, we find that the finite size effects are small at $m_{PS}/m_V = 0.6$, while, at $m_{PS}/m_V = 0.5$, m_V on $16^3 \times 24$ is slightly lower by 2% (1.5σ). A higher statistics is needed to draw more definite conclusions.

Using the data shown in Fig. 4, we test the PCAC relation,

$$\frac{m_{PS}^2}{2B_0 m_q} = 1 + \frac{Cy}{N_f}\log y + \alpha y,\ y \equiv \frac{m_{PS}^2}{(4\pi f_{PS})^2} \quad (1)$$

where B_0 and α are unknown parameters and $C = 1$ from ChPT. Fixing f_{PS} to $f_\pi = 93$ MeV and adopting the AWI quark mass for m_q, the data can be well fitted with $\chi^2/df = 0.05$ when we treat C as a free parameter. However, we obtain $C = 0.06(2)$. Correspondingly, when we fix $C = 1$, the data cannot be described by Eq. (1) ($\chi^2/df \approx 40$). Therefore, our data down to $m_{PS}/m_V = 0.4$ do not show the logarithmic curvature predicted by ChPT.

5. Conclusions

We explored the light quark region of QCD down to $m_{PS}/m_V = 0.4$ using improved Wilson-type quarks. We found that the BiCGStab(DS-L) algorithm is robust at small quark masses. Spikes in ΔH may introduce an additional systematic error but can be suppressed by setting dt small. The origin of the huge quark force is still under investigation. Preliminary analyses on meson masses did not find agreement with the logarithmic behavior expected from chiral perturbation theory to one loop order.

We thank S. Itoh and R. Frezzotti for useful discussions. This work is supported in part by Large Scale Numerical Simulation Project of the Science Information Processing Center, University of Tsukuba, and by Grants-in-Aid of the Ministry of Education (Nos. 11640294, 12304011, 12640253, 12740133,13135204,13640259,13640260,14046202, 14740173). VIL is supported by JSPS.

REFERENCES

1. For a recent review, see T. Kaneko, Nucl. Phys. B (Proc. Suppl.) 94 (2002) 133.
2. H. Wittig, these proceedings.
3. S. Hashimoto, these proceedings.
4. CP-PACS Collaboration: A. Ali Khan *et al.*, Phys. Rev. D65 (2002) 054505.
5. G.L.G. Sleijpen and D.R. Fokkema, Elec. Trans. on Numer. Anal. Vol.1 (1993) 11.
6. T. Miyauchi *et al.*, Trans. of Japan Soc. for Ind. and Appl. Math. Vol.11, No.2 (2001) 49.
7. K. Jansen and R. Sommer, Nucl. Phys. B530 (1998) 185.
8. R.G. Edwards *et al.*, Nucl. Phys. B484 (1997) 375; B. Joó *et al.*, Phys. Rev. D62 (2000) 114501.