Full QCD simulation on CP-PACS

CP-PACS Collaboration:
S. Aoki; G. Boyd; R. Burkhalter; S. Hashimoto; N. Ishizuka; Y. Iwasaki; K. Kanaya; T. Kaneko; Y. Kuramashi; M. Okawa; A. Ukawa; and T. Yoshi
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aInstitute of Physics, University of Tsukuba, Tsukuba, Ibaraki 305, Japan
bCenter for Computational Physics, University of Tsukuba, Tsukuba, Ibaraki 305, Japan
cComputing Research Center, High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305, Japan
dInstitute of Particle and Nuclear Studies, High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305, Japan

A status report is made of an on-going full QCD study on the CP-PACS aiming at a comparative analysis of the effects of improving gauge and quark actions on hadronic quantities and static quark potential. Simulations are made for four action combinations, the plaquette or an RG-improved action for gluons and the Wilson or SW-clover action for quarks, at \(a^{-1} \approx 1.1-1.3\)GeV and \(m_\pi/m_\rho \approx 0.7-0.9\). Results demonstrate clearly that the clover term markedly reduces discretization errors for hadron spectrum, while adding six-link terms to the plaquette action leads to much better rotational symmetry in the potential. These results extend experience with quenched simulations to full QCD.

1. Introduction

With the progress in recent years of quenched simulations of QCD, deviations of the quenched hadron spectrum from experiment are being uncovered. For heavy quark systems precise calculations with NRQCD have shown that the fine structure of quarkonium spectra can be reproduced only if sea quark effects are taken into account [1]. For the light hadron sector several reports have been made that strange quark mass cannot be set consistently from pseudo scalar and vector meson channels in quenched QCD [2,3]. Most recently results of an extensive quenched simulation on the CP-PACS QCD [4,5] indicate that there is a systematic disagreement in the spectrum of baryons [6]. Clearly the time has come to bolster efforts toward full QCD simulations. We have recently started an attempt in this direction using the CP-PACS computer [7].

Full QCD simulations are, however, extremely computer time consuming compared to those of quenched QCD. Even with the TFLOPS-class computers that are becoming available, high statistics studies, indispensable for reliable results, will be difficult for lattice sizes exceeding \(32^3 \times 64\). Since a physical lattice size of \(L \approx 2.5-3.0\)fm is needed to avoid finite-size effects [6,7], the smallest lattice spacing one can reasonably reach will be \(a^{-1} \approx 2\)GeV. Hence lattice discretization errors have to be controlled with simulations carried out at an inverse lattice spacing smaller than this value. This will be a difficult task with the standard plaquette and Wilson quark actions since discretization errors are of order 20-30\% even at \(a^{-1} \approx 2\)GeV [1]. This leads us to consider improved actions for our simulation of full QCD.

Studies of improved actions have been widely pursued in the last few years. Detailed tests of improvement for hadron spectrum, however, have
Table 1: Simulation parameters of full QCD runs on a $12^3 \times 32$ lattice. Numbers in parenthesis denote number of configurations stored for static quark potential analyses.

| $\beta$ | $K$   | $C_{SW}$ | #config | $m_\pi/m_\rho$ |
|--------|-------|----------|---------|----------------|
|        |       |          |         |                |
| **P-W** |       |          |         |                |
| 4.8    | .1846 | 222 (0)  | .83     |                |
|        | .1874 | 200 (0)  | .77     |                |
|        | .1891 | 200 (0)  | .70     |                |
| 5.0    | .1779 | 300 (100)| .85     |                |
|        | .1798 | 301 (101)| .79     |                |
|        | .1811 | 301 (101)| .71     |                |
| **R-W** |       |          |         |                |
| 1.9    | .1632 | 200 (0)  | .90     |                |
|        | .1688 | 200 (0)  | .80     |                |
|        | .1713 | 200 (0)  | .69     |                |
| 2.0    | .1583 | 300 (100)| .90     |                |
|        | .1623 | 300 (100)| .83     |                |
|        | .1644 | 300 (100)| .74     |                |
| **P-C** |       |          |         |                |
| 5.2    | .139  | 208 (100)| .83     |                |
|        | .141  | 207 (100)| .79     |                |
|        | .142  | 200 (100)| .73     |                |
| 5.25   | .139  | 198 (0)  | .83     |                |
|        | .141  | 194 (0)  | .76     |                |
| **R-C** |       |          |         |                |
| 2.0    | .1300 | 201 (191)| .90     |                |
|        | .1370 | 200 (190)| .79     |                |
|        | .1388 | 1515 (138)| .71    |                |

been mostly carried out within quenched QCD (see, e.g., Refs. [12–15]), and only a few studies are available for the case of full QCD [16]. In particular a systematic investigation of how various terms added to the gauge and quark actions, taken separately, affect light hadron observables has not been carried out in full QCD. We have decided to undertake such a study as the first subject of our full QCD program. In this article we report preliminary results of this on-going attempt.

2. Choice of action and simulation parameters

Improving the standard plaquette action for gluons requires the addition of Wilson loops of six links or more in length. The precise forms of the added terms and their coefficients differ depending on the principle one follows for improvement. In our study we choose an action given by

$$S_g^R = \frac{\beta}{6} \left( c_0 \sum W_{1\times 1} + c_1 \sum W_{1\times 2} \right),$$

with $c_0 = 1 - 8c_1$ and $c_1 = -0.331$, which was obtained by a renormalization group treatment [17].

The quenched static quark potential calculated with this action exhibits good rotational symmetry and scaling already at $a^{-1} \approx 1\text{GeV}$ [18], similar to those observed for tadpole-improved and fixed point actions [19,20].

For improving the quark action we take the clover improvement due to Sheikholeslami and Wohlert [21] defined by

$$D_{C_{xy}} = D_{W_{xy}} + \delta_{xy} c_{SW} K \sum_{\mu,\nu} \frac{i}{4} \gamma_{\mu,\nu} F_{\mu,\nu},$$

with the standard Wilson matrix $D_{W_{xy}}$ given by

$$D_{W_{xy}} = \delta_{xy} - K \sum_{\mu} \{ (1 - \gamma_\mu) U_{x,\mu} \delta_{x+\hat{\mu},y} + (1 + \gamma_\mu) U_{x,\mu}^\dagger \delta_{x,y+\hat{\mu}} \}.$$  

For the clover coefficient $c_{SW}$, we adopt the meanfield improved value [22]: $c_{SW} = P^{-3/4}$ with $P$ the plaquette average.

We carry out a comparative study of the light hadron spectrum and static quark potential for four action combinations, choosing either the plaquette (P) or the rectangular action above (R) for gluons and either the Wilson (W) or clover action (C) for quarks. We expect the extent of improvement to be clearer at a coarser lattice spacing. We therefore attempt to tune the coupling constant $\beta$ so that the lattice spacing equals $a^{-1} \sim 1\text{GeV}$.

Our simulations are carried out for two flavors of quarks, mostly on a $12^3 \times 32$ lattice with additional runs on an $8^3 \times 16$ lattice to estimate parameters, including a self-consistent value of $c_{SW}$. We employ the hybrid Monte Carlo algorithm to generate full QCD configurations at two or three values of $K$ corresponding to $m_\pi/m_\rho \approx 0.7-0.9$. The molecular dynamics step size is chosen to yield an acceptance of 80-90%. After thermalizing for 100-200 trajectories we generate 1000-1500 trajectories.
Figure 1. (a) $m_N/m_\rho$ and (b) $m_\Delta/m_\rho$ as a function of $(m_\pi/m_\rho)^2$ for various combinations of the action. Stars in (b) are experimental points corresponding to $\Delta(1232)/\rho(770)$ and $\Omega(1672)/\phi(1020)$.

We measure hadron propagators every 5 trajectories, using point and smeared sources and point sinks following the method of our quenched study [5]. The static quark potential is calculated on a subset of configurations used for hadron propagator measurement. The smearing technique of Ref. [23] is employed choosing the number of smearing steps and fitting ranges from experience in Ref. [18]. Errors are estimated by a single-elimination jackknife procedure. Simulation parameters of our runs and the number of configurations used for the spectrum and potential measurements are summarized in Table 1.

### 3. Light hadron masses

Our main results for the effect of improved actions on hadron masses are displayed in Fig. 1 in which the ratio $m_N/m_\rho$ and $m_\Delta/m_\rho$ are plotted as a function of $(m_\pi/m_\rho)^2$ for the four action combinations. The solid curves represent the well-known phenomenological mass formula [24]. The inverse lattice spacing estimated from the $\rho$ meson mass in the chiral limit is in the range $a^{-1} \approx 1.1-1.3\text{GeV}$ (see Table 2).

Table 2

Results of $a^{-1}$ and $J$ determined by a linear fit of $m_\rho a$ in terms of $(m_\pi a)^2$ using data at $(m_\pi a)^2 \approx 0.3-1.1$ (see discussions in the text). Errors are statistical only.

| action | $\beta$ | $a^{-1}[\text{GeV}]$ | $J$ |
|--------|---------|---------------------|-----|
| P-W    | 4.8     | 1.00(1)             | 0.35(1) |
|        | 5.0     | 1.08(2)             | 0.35(1) |
| R-W    | 1.9     | 1.15(1)             | 0.34(1) |
|        | 2.0     | 1.29(1)             | 0.34(1) |
| P-C    | 5.2     | 1.30(3)             | 0.42(1) |
|        | 5.25    | 1.48(6)             | 0.41(2) |
| R-C    | 2.0     | 1.35(1)             | 0.44(1) |

For the standard action combination P-W, the ratios are well above the phenomenological curve as may be expected at such a large lattice spacing. When we improve the gauge action (the R-W case), the data points come closer to the curve. By far the most conspicuous change, however, is observed when we introduce the clover term to the quark action. For both the P-C and R-C cases, the data points drop significantly and lie on top of the phenomenological curve within errors. The same trend is seen both for $m_N/m_\rho$ and $m_\Delta/m_\rho$.

A similar effect has been observed in quenched QCD by the UKQCD Collaboration in simulations with the P-C combination at $\beta = 5.7-6.2$ ($a^{-1} \approx 1.1-2.5\text{GeV}$) [4], and also in a study with improved gluon actions and the clover and D234 quark actions at coarse lattice spacings of $a^{-1} \approx 0.5-0.7\text{GeV}$ [14]. It is therefore more natural to associate the origin of the effect to valence quarks rather than to dynamical sea quarks in...
full QCD. Nonetheless, changing the gluon and quark actions one at a time, we have been able to see clearly a decisive role played by the clover term in improving the spectrum in a quantitative detail in the context of full QCD. In this regard, improving the gluon action has much less effect.

In Table 2 we compile our results for the $J$ parameter, $J = m_V \frac{d n_V}{d m^2_{PS}}$ at $m_V/m_{PS} = 1.8$. Here again the clover term brings the values into better agreement with the experimental value of 0.48(2).

Another interesting feature in our hadron mass data is that they exhibit a negative curvature in terms of $1/K$ toward the chiral limit. This is in contrast to quenched QCD where hadron masses (mass squared for pseudo scalar mesons) are generally well described by a linear function of $1/K$ up to quite heavy quark. The curvature is reduced if hadron masses are plotted against $m^2_{PS}$, but still remains at a significant level, especially for the R-C combination. This is possibly a full QCD effect due to sea quarks which increasingly ordered gauge configurations toward the chiral limit. For results with clover quark actions the trend may be enhanced by the dependence of $c_{SW}$ on $K$ due to tadpole improvement.

The curvature causes a practical difficulty in the chiral extrapolation of hadron masses since our runs have so far been made with at most three values of $K$. For the estimates of $a^{-1}$ in Table 2 we employed a linear fit of hadron masses in the measured values of $m^2_{PS}$, excluding for the R-C case the point of heaviest quark mass.

In this connection we note that a comparison such as in Fig. 1 and for $J$ in Table 2 should be made at the same lattice spacing in physical units. As we see in Table 2 our estimate of $a^{-1}$ shows a spread of some 20-30% depending on the actions. Additional runs are being conducted in an effort to match the lattice spacing more precisely.

Another point to note is that an agreement with the phenomenological formula of Ref. [2]
examined in Fig. 1 is not an improvement criterion that follows from theoretical principles, albeit a reasonable one in view of the success of the formula for describing the experimental spectrum. Stability of results toward smaller lattice spacing has to be checked, which we hope to pursue in future simulations.

4. Static quark potential

We plot typical results for the static quark potential in Fig. 2 for which \( m_\pi/m_\rho \approx 0.8 \). Conversion to physical units is made with the lattice scale given in Table 2. Different symbols correspond to potential data measured in different spatial directions along the vector given in the figure.

For the P-W action rotational symmetry is badly violated. Improving the quark action (P-C) we observe that the potential exhibits a much better rotational symmetry. At present how much of the improvement is due to the change of the quark action is not clear since the lattice spacing for the P-C case \( a^{-1} \approx 1.3 \text{GeV} \) is about 20% smaller than for the case of P-W \( a^{-1} \approx 1.1 \text{GeV} \), from which one expects a 40% reduction in the violation of rotational symmetry. The best improvement is achieved with the R-W and R-C actions. It is known that the gauge action R significantly improves rotational symmetry already for the quenched case [18]. The improvement naturally carries over to the present case of full QCD.

With our present statistics the potential can be measured with small errors up to a distance of \( r \approx 6a \approx 1 \text{fm} \). In this distance range we do not observe flattening of the potential due to pair creation and annihilation effects. In fact the potential can be well described by a linear plus Coulomb form \( \sigma r + \alpha/r \). We extract the string tension \( \sigma \) by fitting potential data to this form. We then use the phenomenological value \( \sigma = (440 \text{MeV})^2 \) to convert results to an estimate of \( a \) for each value of \( K \).

In Fig. 3 we compare the value of \( a \) obtained...
in this way (filled circles) with that from \( m_\rho = 770\text{MeV} \), also calculated for each value of \( K \) (open circles). For the latter quantity, results obtained after an extrapolation of \( m_\rho a \) to the chiral limit are also shown. This extrapolation is linear for \( a \) when we take \( (m_\pi a)^2 \) as the horizontal axis, as adopted in Fig. 3. We observe that the two estimates converge to a consistent value in the chiral limit for the P-C and R-C combinations, while an apparent deviation of order 40\% and 20\% are indicated for the cases of P-W and R-W respectively.

Of course we expect the discrepancy observed for the last two cases with the Wilson quark action to disappear in the continuum limit. The agreement found for the P-C and R-C cases show that the clover term helps improve the consistency of the two determinations of the physical scale of lattice spacing already at \( a^{-1} \approx 1.3\text{GeV} \).

The static quark potential at short distances is directly relevant to the spectrum of heavy quark systems. A recent NRQCD calculation carried out on gauge configurations generated with the Kogut-Susskind action for sea quark and the plaquette gluon action at \( \beta = 5.6 \) shows a significant deviation between the scale determined from the heavy and light hadron spectrum[11]. It would be interesting to check for our P-C and R-C cases if the lattice scale determined from heavy quark systems yield results consistent with those from \( \sigma \) and \( m_\rho \).

5. Conclusions

Our comparative study has shown that the clover term of Sheikholeslami and Wohlert drastically improves light hadron spectrum already at \( a^{-1} \approx 1.1-1.3\text{GeV} \). While improving the gauge action has much less effect in this regard, we expect good rotational symmetry of static quark potential, which is achieved with the action R, to be important for heavy quark systems.

Our results lead us to believe that a significant step forward towards a realistic simulation of full lattice QCD, encompassing both heavy and light hadrons, can be achieved with the current generation of dedicated parallel computers with the application of improved actions. We are particularly encouraged to pursue the use of the combination R-C toward this goal.

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REFERENCES

1. C.T.H. Davies et al., Phys. Lett. B345 (1995) 42; C.T.H. Davies, these proceedings.
2. P. Lacock and C. Michael, Phys. Rev. D52 (1995) 5213.
3. T. Bhattacharya et al., Phys. Rev. D53 (1996) 6486.
4. R. Kenway for UKQCD Collaboration, Nucl. Phys. B (Proc. Suppl.) 53 (1997) 206.
5. CP-PACS Collaboration (presented by T. Yoshié), these proceedings.
6. See, however, R. Kenway, these proceedings.
7. Y. Iwasaki, these proceedings.
8. M. Fukugita et al., Phys. Rev. D47 (1993) 4739; S. Aoki et al., ibid. D50 (1994) 486.
9. S. Gottlieb, these proceedings; Nucl. Phys. B (Proc. Suppl.) 53 (1997) 155.
10. F. Butler et al., Nucl. Phys. B421 (1994) 217.
11. J. Sloan, these proceedings.
12. M. Alford et al., Phys. Lett. B361 (1995) 87; G. P. Lepage, these proceedings.
13. S. Collins et al., Nucl. Phys. B(Proc. Suppl.) 47 (1996) 378; ibid. 53 (1997) 877.
14. W. Bock, Nucl. Phys. B(Proc. Suppl.) 53 (1997) 870.
15. C. Bernard et al., Nucl. Phys. B (Proc. Suppl.) 53 (1997) 212.
16. S. Collins et al., Nucl. Phys. B (Proc. Suppl.) 47 (1996) 378; ibid. 53 (1997) 880.
17. Y. Iwasaki, Nucl. Phys. B258 (1985) 141; Univ. of Tsukuba report UTHEP-118 (1983), unpublished.
18. Y. Iwasaki et al., Nucl. Phys. B (Proc. Suppl.) 53 (1996) 429; Phys. Rev. D56 (1997) 151.
19. M. Alford, W. Dimm, and G.P. Lepage, Nucl. Phys. (Proc. Suppl.) 42 (1995) 787.
20. T. DeGrand et al., Nucl. Phys. B454 (1995) 615.
21. B. Sheikholeslami and R. Wohlert, Nucl. Phys. B259 (1985) 572.
22. G.P. Lepage and P.B. Mackenzie, Phys. Rev. D48 (1993) 2250; P.B. Mackenzie, Nucl. Phys. B (Proc. Suppl.) 30 (1993) 35.
23. G.S. Bali and K. Schilling, Phys. Rev. D46 (1992) 2636.
24. S. Ono, Phys. Rev. D17 (1978) 888.