Large-scale simulations with chiral symmetry

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We carry out a comparative study among five-dimensional formulations of chirally symmetric fermions about the algorithmic performance, chiral symmetry violation and topological tunneling to find a computationally inexpensive formulation with good chiral symmetry. With our choice of the lattice action, we have launched large-scale simulations on fine lattices aiming at a precision study of light and heavy quark physics. We report on the comparative study, current status of the large-scale simulations, and preliminary results on the residual quark mass and auto-correlation.

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1. Introduction

In the last several years, we performed an extensive study of QCD vacuum and light hadron physics by using the overlap action which exactly preserves chiral symmetry \[1\]. Our next target is a precision study of heavy flavor physics in collaboration with flavor factory experiments, such as the SuperKEKB / Belle II experiment, for a stringent test of the Standard Model.

Since the overlap action is computationally too expensive to simulate small lattice spacings \(a \ll m_{c}^{-1}\) on reasonably large lattices, we carried out a systematic comparative study of a class of five-dimensional formulations that approximately satisfy the Ginsparg-Wilson relation to construct a computationally cheap formulation with good chiral symmetry. In this article, we report on the comparative study and the status of the on-going large-scale simulations with our choice of the lattice action.

2. Comparative study

We test five-dimensional fermion formulations \[2\] in this comparative study. The four-dimensional effective Dirac operator is given by

\[
\frac{1 + m_q}{2} \gamma_5 \varepsilon_M(H_M),
\]

where the Hermitian kernel operator \(H_M\) and the approximation of its sign function \(\varepsilon_M\) can be chosen by tuning parameters appearing in the five-dimensional Dirac operator. Popular choices of \(H_M\) are the Wilson kernel \(H_W = \gamma_5 D_W\), where \(D_W\) is the Wilson-Dirac operator, for the overlap fermions, and the Shamir kernel \(H_T = \gamma_5 D_W / (2 + D_W)\) for the standard domain-wall fermions. We also test a scaled Shamir kernel \(2H_T\) \[2\]. While \(2H_T\) has the same condition number as \(H_T\), its low-lying eigenvalues are scaled up by a factor of 2. These kernels are combined with the Zolotarev (\(\varepsilon_Z\)) and polar decomposition (\(\varepsilon_p\)) approximations. By applying up to 6 level stout smearing \[3\] \((N_{\text{smr}} = 0, 3, 6)\), we test 8 different formulations listed in Table 1.

Table 1: Simulation setup in our comparative study. The first three columns show our choices of the five-dimensional formulation: the number of smearing \(N_{\text{smr}}\), kernel operator \(H_M\) and sign function approximation \(\varepsilon_M\). We also list simulation parameters, namely \(\beta\) and the bare quark mass in lattice units \(a m_{ud}\), as well as results for \(a^{-1}\) and \(M_{\pi}\).

| \(N_{\text{smr}}\) | \(H_M\) | \(\varepsilon_M\) | \(\beta\) | \(a^{-1}\) [GeV] | \(a m_{ud}\) | \(M_{\pi}\) [MeV] |
|---------------|-----------|----------------|---------|----------------|----------------|----------------|
| 0             | \(H_W\)   | \(\varepsilon_Z\) | 4.27    | 1.98(6)        | 0.0095, 0.0060, 0.0035 | 463(17), 375(17), 346(25) |
| 0             | \(H_T\)   | \(\varepsilon_Z\) | 4.11    | 1.92(6)        | 0.0200, 0.0120, 0.0065 | 543(18), 419(15), 318(15) |
| 0             | \(H_T\)   | \(\varepsilon_p\)| 4.11    | 1.97(5)        | 0.0200, 0.0090, 0.0040 | 623(19), 483(16), 400(15) |
| 0             | \(2H_T\)  | \(\varepsilon_p\)| 4.11    | 1.94(6)        | 0.0200, 0.0120, 0.0065 | 554(18), 434(17), 356(16) |
| 3             | \(H_W\)   | \(\varepsilon_Z\) | 4.29    | 1.94(6)        | 0.0145, 0.0090, 0.0050 | 472(18), 401(17), 330(17) |
| 3             | \(H_T\)   | \(\varepsilon_p\)| 4.18    | 2.00(8)        | 0.0250, 0.0170, 0.0090 | 534(23), 423(20), 374(23) |
| 3             | \(2H_T\)  | \(\varepsilon_p\)| 4.18    | 2.06(9)        | 0.0250, 0.0170, 0.0090 | 524(24), 469(24), 364(25) |
| 6             | \(2H_T\)  | \(\varepsilon_p\)| 4.18    | 2.11(6)        | 0.0250, 0.0170, 0.0090 | 511(17), 430(16), 337(20) |
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Figure 1: Left panel: number of MD steps $N_{\text{MD}, P=0.80}$ to attain 80% acceptance rate. Data for different formulations are plotted in different symbols as a function of $M_{\pi}^2$. Right panel: CG iteration count $N_{\text{inv}}$ as a function of $M_{\pi}^{-2}$.

Figure 2: A measure of CPU cost per HMC trajectory $N_{\text{MD}, P=0.80} N_{\text{inv}}$. The left panel shows all data, whereas the right panel is an enlargement of a region of small $N_{\text{MD}, P=0.80} N_{\text{inv}}$ to focus on computationally cheaper formulations.

We carry out numerical simulations of two-flavor QCD by using these formulations and the tree-level Symanzik gauge action to study the performance of the Hybrid Monte Carlo (HMC) algorithm, chiral symmetry violation and topological tunneling. On a $16^3 \times 32$ lattice, we simulate three pion masses in the range of $300 \lesssim M_{\pi}[\text{MeV}] \lesssim 600$ at a single lattice cut-off around $a^{-1} \simeq 2$ GeV. The fifth dimensional size is set to $N_5 = 12$. We set the range of the Zolotarev approximation $\varepsilon_{\varepsilon}(x)$ to $x \in [0.2, 7.0]$ ($[0.4, 7.0]$) for $H_W$ without (with) smearing, and $[0.1, 1.5]$ for $H_T$. Our statistics are 1,000 trajectories in each simulation. Parameters and results for $a^{-1}$ and $M_{\pi}$ are summarized in Table 1, where $r_0 = 0.462(11)/4$ fm [4] is used as input to fix $a$.

In each simulation, we keep the acceptance rate of $P \simeq 0.7 - 0.9$ using a moderately small step size $\Delta \tau$ for the Molecular Dynamics (MD) integration. The number of the MD steps to attain a reference value $P = 0.8$, which is denoted by $N_{\text{MD}, P=0.80}$ in the following, is estimated from the relations holding at small $\Delta \tau$

$$P = \text{erfc} \left( \frac{1}{2} \sqrt{\Delta H} \right), \quad \langle \Delta H \rangle \propto \Delta \tau^4, \quad (2.2)$$

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where $\langle \Delta H \rangle$ represents the Monte Carlo average of the change of the Hamiltonian due to the discretized MD integration. Figure 1 compares $N_{\text{MD}, p=0.80}$ and the iteration count for CG per MD step, denoted by $N_{\text{inv}}$, among the tested formulations. We observe that these two measures of the CPU cost significantly decrease by i) switching from $H_W$ to (2)$H_T$, ii) switching from $\epsilon_Z$ to $\epsilon_p$, and iii) applying smearing ($N_{\text{smr}} \geq 3$). On the other hand, there is no large difference in these measures between Shamir-type kernels ($H_T$ and $2H_T$) and between $N_{\text{smr}} = 3$ and 6.

The product $N_{\text{MD}, p=0.80}N_{\text{inv}}$ can be considered as a measure of the CPU cost per HMC trajectory. As plotted in Fig. 2, the overlap formulation, namely the combination of $H_W$ and $\epsilon_Z$, turns out to be computationally very demanding. We can achieve about a factor of 20 acceleration at $M_\pi \approx 400$ MeV: a factor of 5 by using (2)$H_T$ and $\epsilon_p$, and an additional factor of 4 by smearing. We may expect even bigger gain at smaller quark masses.

These computationally cheaper formulations are, however, off from practical use, if they largely violate chiral symmetry. We compare residual quark mass $m_{\text{res}}$ in Fig. 3. Since the min-max approximation can satisfy $|\epsilon_Z(x)|^2 \sim 1$ in its approximation range, $\epsilon_Z$ leads to the least $m_{\text{res}}$ at a given $N_{\text{smr}}$. With our choice of $N_S = 12$, however, $|\epsilon_p(x)|^2$ largely deviates from unity at $x \lesssim 0.3$,
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Table 2: Status of our simulations at \( a^{-1} \approx 2.4 \) GeV. The third column shows the choice of the MD integrator, namely the leap-frog (LF) or Omelyan (O) integrator. We also list time per HMC trajectory on the whole machine of BlueGene/Q at KEK in the last column.

| \( am_{ud} \) | \( am_s \) | MD | \( N_{MD} \) | traj | \( P \) | \( \langle \Delta H \rangle \) | \( \langle e^{-\Delta H} \rangle \) | min/traj |
|---|---|---|---|---|---|---|---|---|
| 0.019 | 0.040 | LF | 10 | 3000 | 0.78(1) | 0.19(1) | 0.99(1) | 2.7 |
| 0.012 | 0.040 | LF | 13 | 2000 | 0.78(1) | 0.17(1) | 1.00(1) | 3.5 |
| 0.012 | 0.040 | O | 3 | 1000 | 0.89(1) | 0.07(2) | 1.01(1) | 2.0 |
| 0.007 | 0.040 | LF | 16 | 1000 | 0.74(1) | 0.23(2) | 1.04(1) | 4.4 |
| 0.007 | 0.040 | O | 4 | 2000 | 0.90(1) | 0.06(1) | 1.00(1) | 2.6 |
| 0.019 | 0.030 | LF | 10 | 3000 | 0.79(1) | 0.17(1) | 1.00(1) | 2.8 |
| 0.012 | 0.030 | LF | 13 | 2000 | 0.79(1) | 0.14(1) | 1.02(1) | 3.6 |
| 0.012 | 0.030 | O | 3 | 1000 | 0.88(1) | 0.10(3) | 1.00(1) | 2.0 |
| 0.007 | 0.030 | LF | 16 | 2000 | 0.72(1) | 0.27(2) | 1.00(2) | 4.5 |
| 0.007 | 0.030 | O | 4 | 1000 | 0.89(1) | 0.08(2) | 0.99(1) | 2.6 |

where thin-link kernels have many low-lying modes as shown in Fig. 3. Scaling of the kernel \((H_T \rightarrow 2H_T)\) and smearing \((N_{smr}=3)\) are very effective to suppress these low-lying modes leading to an order of magnitude smaller \(m_{res}\) compared to the standard domain-wall fermions. Larger \(N_{smr}\) is better in reducing \(m_{res}\) but may distort short distance physics. We refer to Ref. [5] for more detailed discussions.

Figure 4 shows examples of the Monte Carlo history of the topological charge \(Q\). A low-lying eigenvalue flips its sign along a tunneling between topological sectors. While scaling and smearing suppress the low-lying modes, the comparison in Fig. 4 suggests that these techniques do not prevent the topological tunneling at \(a^{-1} \approx 2\) GeV.

From this comparative study, we conclude that the combination of \(2H_T\) and \(\varepsilon_p\) with \(N_{smr}=3\) is the best choice among the tested formulations.

3. Large-scale simulations

We have launched large-scale simulations of \(N_f = 2+1\) QCD with good chiral symmetry, namely with \(m_{res}\) well below the physical up and down quark mass \(m_{ud,phys}\). The tree-level Symanzik gauge action is combined with the fermion formulation chosen by the comparative study to be consistent with our \(O(a^2)\)-improvement program for heavy quark physics [6]. For controlled continuum and chiral extrapolations, we are planning to simulate the pion masses of 500, 400, 300 MeV (and even smaller) at four values of the lattice cut-off \(a^{-1} \approx 2.4, 3.0, 3.6\) and 4.8 GeV. Finite volume effects are suppressed to 1–2% level by keeping \(M_\pi L \gtrsim 4\). These simulations are being carried out on BlueGene/Q at KEK (6 racks with a peak speed of 1.258 PFLOPS).

Table 2 shows the current status of our simulations on a \(32^3 \times 64 \times 12\) lattice at \(\beta = 4.17\), where \(a^{-1}\) determined from \(r_0\) is expected to be \(\approx 2.4\) GeV. The three values of the bare light quark mass \(m_{ud}\) correspond to \(M_\pi \approx 500, 400\) and 300 MeV, whereas we take two strange quark masses \((m_s’\)s) near its physical value \(m_{s,phys}\). We employ the Hasenbusch preconditioning [7] with the mass parameter \(am' = 0.150\) for two degenerate light flavors, and the rational HMC algorithm [8] for the

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Table 3: Status of our simulations at $a^{-1} \simeq 3.6$ GeV.

| $am_{ud}$ | $am_s$ | $am'$ | $N_{MD}$ | traj | $P_{HMC}$ | $\langle \Delta H \rangle_{\min/\text{traj}}$ |
|----------|-------|------|---------|------|----------|------------------|
| 0.0120   | 0.0250| 0.10 | 4       | 430  | 0.84(2)  | 0.10(2) 3.6      |
| 0.0080   | 0.0250| 0.08 | 4       | 330  | 0.85(2)  | 0.06(2) 4.2      |
| 0.0042   | 0.0250| 0.04 | 4       | 235  | 0.92(3)  | 0.04(2) 5.9      |
| 0.0120   | 0.0180| 0.10 | 4       | –    | –        | –                 |
| 0.0080   | 0.0180| 0.08 | 4       | 260  | 0.86(1)  | 0.05(1) 4.3      |
| 0.0042   | 0.0180| 0.04 | 4       | 280  | 0.86(3)  | 0.02(2) 6.0      |

single strange flavor. We had started our simulations with the simple leap-frog MD integrator, which was later switched to the Omelyan integrator \[9\] leading to a factor of 2 speed-up. We keep reasonably high acceptance rate $P \simeq 0.7 - 0.9$ and confirm that $\langle e^{-\Delta H} \rangle = 1$ derived from the area preserving property of HMC is well satisfied.

We are also carrying out simulations at a larger lattice cut-off $a^{-1} \simeq 3.6$ GeV ($\beta = 4.35$) on $48^3 \times 96 \times 8$. The current status is summarized in Table 3. We increase the unit trajectory length to $\tau = 2$ based on our preparatory study on the auto-correlation (see below). Our choice of the fermion action as well as careful tuning of $m'$ at each $m_{ud}$ enable us to achieve the high acceptance rate $P \gtrsim 0.85$ with small $N_{MD} = 4$. We expect half a year to accumulate 10,000 MD time on this large volume by using BlueGene/Q at KEK. This will be accelerated by further optimization of our simulation code \[10\].

We plot $m_{res}$ from these simulations in Fig. 5, where the renormalization factor to the $\overline{\text{MS}}$ scheme at 2 GeV is roughly estimated by matching our estimate of the bare value of $m_{s,phys}$ with a world average \[11\] in that scheme. It turns out that $m_{res} \simeq 0.5$ MeV at $a^{-1} \simeq 2.4$ GeV with $N_5 = 12$. At $a^{-1} \simeq 3.6$ GeV, $m_{res}$ is even smaller ($\simeq 0.1$ MeV) with smaller $N_5 = 8$. While these $m_{res}$'s are already much smaller than $m_{ud,phys}$, we are considering to further reduce $m_{res}$ by reweighting \[12\].

In Fig. 6, we compare the topological tunneling at $a^{-1} \sim 2.4$ and 3.6 GeV. The auto-correlation largely increases by approaching the continuum limit with the unit trajectory length $\tau$ held fixed. As suggested in Ref. \[13\], we observe that topology changes more frequently with larger $\tau$ in our study in quenched QCD at a similar cut-off $a^{-1} \simeq 3.5$ GeV. This observation leads us to increase $\tau$ when exploring $a^{-1}$ above 2.4 GeV to accelerate our Monte Carlo sampling of topological sectors.

In this article, we reported on our new project of large-scale simulations of $N_f = 2+1$ QCD with good chiral symmetry. The lattice action is chosen by the comparative study to reduce $m_{res}$ well below the physical quark masses and achieve a factor of 20 acceleration compared to the overlap formulation. We are planning to accumulate high statistics of 10,000 MD time for a precision study.
of QCD. Our preliminary results on the light hadron physics were presented at this conference [14].

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