

Dynamical overlap fermion at fixed topology

**JLQCD collaboration: S. Hashimoto^{*,a,b,†}, S. Aoki^c, H. Fukaya^d, K. Kanaya^c,
T. Kaneko^{a,b}, H. Matsufuru^a, M. Okamoto^a, T. Onogi^e, N. Yamada^{a,b}**

^a High Energy Accelerator Research Organization (KEK), Tsukuba 305-0801, Japan

^b School of High Energy Accelerator Science, the Graduate University for Advanced Studies (Sokendai), Tsukuba 305-0801, Japan

^c Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan

^d Theoretical Physics Laboratory, RIKEN, Wako 351-0198, Japan

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

We launched a project to perform dynamical fermion simulations using the overlap fermion formulation for sea quarks. In order to avoid the appearance of near-zero modes of the hermitian Wilson-Dirac operator H_W , we introduce a pair of extra Wilson fermions with a large negative mass term. Crossing of the topological boundary is then strictly prohibited, and the topological charge is conserved during simulations. It makes the simulations substantially faster compared to the algorithms which allow for a change in topological charge. We discuss the finite volume effects due to the fixed global topology.

XXIV International Symposium on Lattice Field Theory
July 23-28 2006
Tucson Arizona, US

*Speaker.

†E-mail: shoji.hashimoto@kek.jp

1. Introduction

The JLQCD collaboration launched a new project to perform dynamical fermion simulations with exact chiral symmetry using the overlap fermion formulation for sea quarks. It allows us to realize exact simulations of the chiral symmetry breaking phenomena starting from the first principles. With the exact chiral symmetry there is no fundamental difficulty to simulate arbitrarily light quarks, which is essential for the controlled chiral extrapolation of many important physical quantities, such as the meson decay constants, bag constants, form factors, and so on. This talk is one of the first reports of our project [1, 2, 3, 4], which makes use of the new supercomputer system (Hitachi SR11000 and IBM BlueGene/L) installed at KEK in March 2006.

2. Extra Wilson fermions

The whole numerical difficulty of the overlap fermion comes from the matrix sign function included in the definition of the overlap-Dirac operator [6]

$$D = m_0 [1 + \gamma_5 \text{sgn}(aH_W)], \quad (2.1)$$

where H_W stands for the hermitian Wilson-Dirac operator $H_W = \gamma_5 D_W(-m_0)$ with large negative mass $am_0 = 1.6$. One usually employs polynomial or rational function to approximate the sign function, which becomes increasingly difficult when there are many near-zero eigenmodes of H_W . Furthermore, the molecular dynamics Hamiltonian in the HMC simulation involves discontinuity when the near-zero mode pass through zero. Such discontinuity may be treated exactly using the so-called “reflection/refraction” trick introduced by Fodor, Katz, and Szabo [5], but its numerical cost scales at least as $\sim V^2$ as the lattice volume V increases, and the simulation on reasonably large lattices, *e.g.* $16^3 \times 32$ as used in our work, becomes prohibitively costly.

The near-zero modes of H_W appear on rough gauge configurations. In fact, the corresponding eigenvector develops a local lump, *i.e.* an exponentially localized wave function with support length as small as a few lattice sites [7, 8, 9, 2]. The net topological charge of the gauge field as defined through the index of D can change its value only through such rough gauge configurations. It implies that the problem of near-zero modes is one of the lattice artifacts disappearing in the continuum limit. A relevant question is, then, whether such artifacts can be removed at finite lattice spacings by choosing lattice action appropriately.

In fact, one may construct a class of lattice actions for which the exact zero mode is prohibited by introducing extra Wilson fermions with a large negative mass $-m_0$ [10, 11, 12]. For the two-flavor case it produces a determinant factor $\det H_W^2$ which suppresses near-zero modes of H_W and strictly prohibits the appearance of exact zero modes. In the continuum limit, the extra fermions become irrelevant as they have a mass of order of lattice cutoff.

We also add a pair of twisted mass pseudo-fermions in order to cancel the unwanted effects of the extra fermions for higher modes. Namely, we introduce a determinant factor $\det[H_W^2 / (H_W^2 + \mu^2)]$ with μ a twisted mass. Since the effect on higher modes is largely cancelled in the ratio, the finite renormalization of the parameters can be minimized. For instance, the β -shift, necessary change of the β value to keep the same lattice spacing, is 0.786(4) without pseudo-fermions, but is reduced to 0.050(1) with the pseudo-fermions with twisted mass $\mu = 0.2$ [12].

The numerical evidences of the effect of the extra Wilson fermions are extensively studied in the quenched approximation (in the sense that the dynamical overlap fermion is not included) and presented in [12, 2]. To be short, the problematic near-zero modes essentially disappear while keeping the β -shift minimal.

3. Dynamical overlap fermions

Our methods for simulating dynamical overlap fermions are rather standard except for the introduction of extra Wilson fermions as discussed above.

We approximate the sign function using the rational function with Zolotarev coefficients. Lowest-lying modes below some threshold are treated exactly. With (typically) 10 poles for the rational function we keep the precision of the sign function to the level of $10^{-(7-8)}$. For the solver of the overlap-Dirac operator we use the conjugate gradient algorithm with relaxed precision [13]. In the inner loop for the rational function calculation, we use the multi-shift CG algorithm. (More recently, we tested a five dimensional implementation of the overlap solver [14] and found it is about $\times 4$ faster. The details are discussed in [4].)

In the molecular dynamics evolution we introduce the Hasenbusch's mass preconditioner [15] with multi-time steps: (1) inner-most loop containing gauge and Wilson fermion forces, (2) middle loop treating the mass preconditioner (Hasenbusch) for the overlap fermion, and (3) outer loop with preconditioned overlap fermion.

The numerical simulations described in this talk have been done on a $16^3 \times 32$ lattice. We use the Iwasaki gauge action. The twisted mass μ of the extra psuedo-fermions is fixed to 0.2. The β value is chosen such that the lattice spacing determined through r_0 becomes 0.11–0.12 fm. As a result we have two series of runs at $\beta = 2.35$ ($a = 0.11$ fm) and at $\beta = 2.30$ ($a = 0.12$ fm). In both cases we performed simulations at six values of quark masses corresponding to $m_s/6 - m_s$. Our main data are those of $\beta = 2.30$, whose analysis is discussed in more detail in [1], while the $\beta = 2.35$ run has been performed for parameter tuning. At $\beta = 2.35$, we also carried out a test run in the ε -regime: quark mass is so small (in our test run, ~ 2 MeV) that $m_\pi L \ll 1$. Its analysis is described in [3]. The topological charge is fixed to 0 for all runs.

For a comparison, we also implemented the reflection/refraction steps and carried out a test run at $\beta = 2.45$ with a relatively heavy sea quark mass ($\sim m_s$). In this case we switched off the extra Wilson fermions.

Here we discuss the effect of the extra Wilson fermion in the molecular dynamics evolution. In Figure 1 we plot the HMC history of the maximum molecular dynamics force (left) and the lowest-lying eigenvalues of H_W (right). The force term is calculated at each step of the molecular dynamics evolution and its maximum value over the whole lattice sites is plotted on the left panel. We clearly see a hierarchy “gauge” \gg “preconditioner” \gg “preconditioned”, justifying our choice of the multi-time steps. Among other forces, that from the extra Wilson fermions (plus psuedo-fermions) has the largest fluctuation, and sometimes becomes larger than the gauge force. This is the reason that we include this force calculation in the inner-most loop together with the gauge force. The right panel shows how the extra Wilson fermions repel the near-zero eigenvalues. There are quite a few cases where the lowest eigenvalue tries to accross zero, but it is bounced back by the

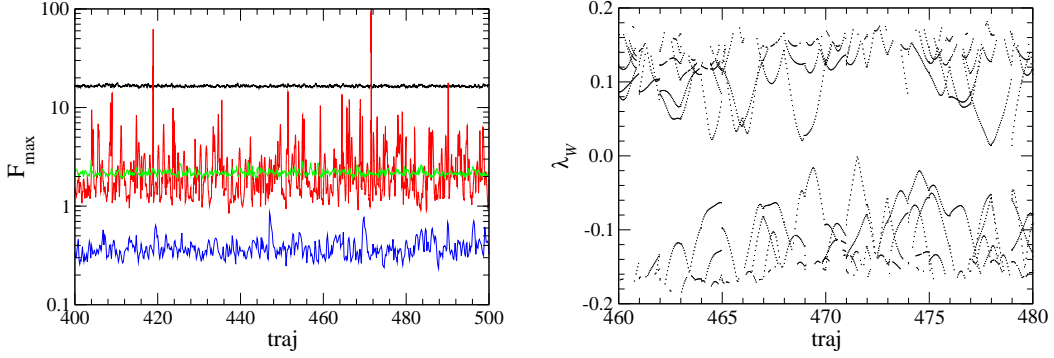


Figure 1: Left: History of maximum molecular dynamics force for gauge (black), extra Wilson fermion (red), preconditioner overlap (green), and preconditioned overlap (blue). Right: History of lowest-lying eigenvalues of H_W . Data at $\beta = 2.35$ and $am = 0.110$.

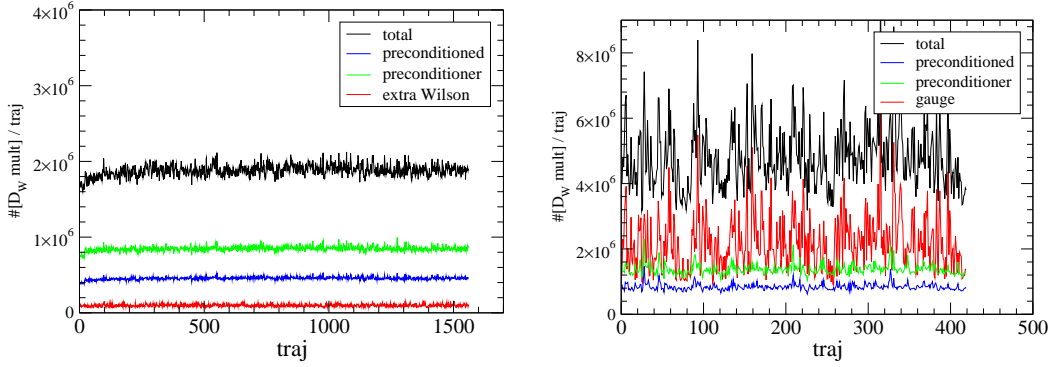


Figure 2: Numerical cost per trajectory measured by the number of the Wilson-Dirac operator multiplication. Left: the cost with the extra Wilson fermions. Right: the cost without the extra Wilson fermions but with the reflection/refraction steps. In addition to the total cost (black), its breakdown to preconditioned overlap (blue), preconditioner overlap (green) and extra Wilson (red) are shown. On the right panel, the red shows the cost for gauge steps including the reflection/refraction. Data at $\beta = 2.35$ and $am = 0.110$ (left) and at $\beta = 2.45$ and $am = 0.090$ (right).

repulsive force. As a result, the net topological charge never changes its value during the molecular dynamics evolutions.

Although the extra Wilson fermions are put in the inner-most loop and they require a solver of the Wilson fermion at every steps, their numerical cost is not substantial. Figure 2 shows the breakdown of the numerical cost per HMC trajectory. As plotted in the left panel, we find that the cost for the extra-Wilson fermion is several times smaller than that for the overlap fermion forces and is only about 5% of the total cost. The right panel, on the other hand, shows the cost with the reflection/refraction steps. We can see that about a half (or more) of the total numerical cost is spent for the gauge steps, which contain the monitoring of the lowest-lying eigenvalues at the every steps and the reflection/refraction when they tend to across zero. Once the reflection/refraction steps are entered, two inversions of the overlap operator are required, and this is the reason why the cost is fluctuating very much. Not just the fluctuation but the average magnitude is more than a factor of two larger than the case with the extra Wilson fermions (and thus without reflection/refraction).

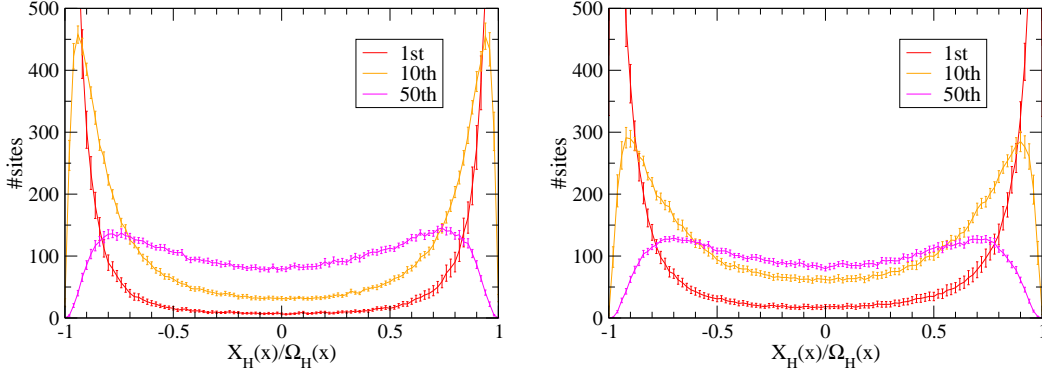


Figure 3: Correlation of the density $\Omega_i(x) = \psi_i^\dagger(x)\psi_i(x)$ and chiral density $X_i(x) = \psi_i^\dagger(x)\gamma_5\psi_i(x)$. Results for the lowest, 10th, and 50th eigenvalues are shown after averaging over 50 gauge configurations. Data are for a quenched lattice at $\beta = 2.37$ (left) and for a dynamical run at $\beta = 2.35$, $am = 0.110$ (right).

Furthermore, we expect that the cost for reflection/refraction increases as V^2 as the lattice volume V increases and becomes a limiting factor in larger volume simulations. This is the reason that we do not take this option in our main runs.

4. Topology issues

The advantage of the fixed topology simulation with the extra Wilson fermion is not just its lower numerical cost, but it suppresses a certain class of discretization effects coming from dislocations. An obvious disadvantage, on the other hand, is the fixed topological charge during the HMC simulations, which implies that the correct $\theta = 0$ vacuum can not be sampled.

In this project we rely on the cluster decomposition property of the local field theory, which suggests that the global topology is irrelevant for local physics as far as the volume is large enough. Our expectation is that the topological fluctuations are active in local areas of the lattice, even though the global topology is fixed. The topological susceptibility χ_t controls the frequency of the local fluctuations. In the instanton picture of the QCD vacuum, the local topological fluctuation could occur through an instanton-anti-instanton pair creation. Once an instanton, which is a local object, is created, it may move around the lattice until it meets an anti-instanton to pair annihilate. The local topological fluctuation should then manifest itself in the space-time distribution of associated local zero modes, which would become localized near-zero modes when measured on the whole lattice.

As a demonstration we look at the correlation between the density $\Omega_i(x) = \psi_i^\dagger(x)\psi_i(x)$ and chiral density $X_i(x) = \psi_i^\dagger(x)\gamma_5\psi_i(x)$ of the low-lying eigenvectors $\psi_i(x)$ of the overlap-Dirac operator. Here, i labels different eigenvectors. As found in the previous works [16, 17, 18], the distribution of the ratio $X_i(x)/\Omega_i(x)$ peaks at ± 1 when the local lumps of the eigenmode $\psi_i(x)$ are predominantly chiral. (We put a cut on $\Omega_i(x)$ such that only the points satisfying $\Omega_i(x) > 1/V$ are counted.) Figure 3 shows our results for quenched (left) and dynamical (right) lattices. The global topology is fixed to 0 on both lattices. The double peak structure is clearly seen especially for the lowest-lying eigenmode on both lattices. This result supports our expectation that there are local topological lumps even in the fixed topology simulations.

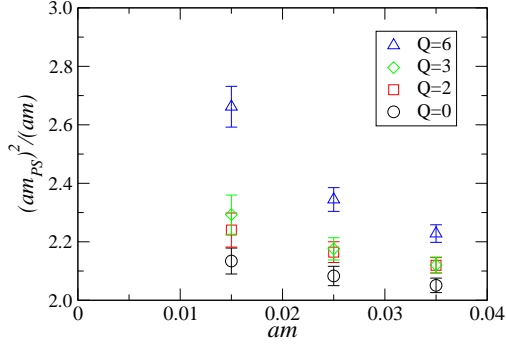


Figure 4: m_{PS}^2/m_q for different topological charges $Q = 0, 2, 3, 6$.

Hadron masses calculated at a fixed topological charge may deviate from their values in the $\theta = 0$ vacuum. Within the framework of chiral lagrangian it is possible to calculate such effects [19]. The difference is predicted as $M''(0)/(2\langle Q^2 \rangle) (1 - Q^2/\langle Q^2 \rangle)$, where $M''(0)$ is a second derivative of the relevant hadron mass with respect to θ . Since $\langle Q^2 \rangle = \chi_t V$ appears in the denominator, the deviation behaves as $1/V$. Although the effect becomes larger for smaller quark masses (for small enough m one expects $\chi_t = m\Sigma/N_f$), the size is $O(1\%)$ on our smallest quark mass, for which the pion mass is around 300 MeV.

As a first test we compare the pion mass calculated in the quenched approximation at several fixed topological charges. On a $16^3 \times 32$ lattice at $\beta = 2.37$ ($a \simeq 0.125$ fm), we have carried out quenched simulations with the extra Wilson fermion, starting from gauge configurations with definite topological charges $Q = 0, 2, 3$ and 6 . For each Q we accumulate 100 gauge configurations each separated by 200 HMC trajectories and measure pion masses. From the results in the quenched continuum limit [20] we expect the average topological charge squared on our lattice to be $\langle Q^2 \rangle = 33(3)$, which leads to an expectation of fairly small effect $\sim O(0.2\%)$ at the tree level of chiral effective theory.

The results for $(am_{PS})^2/(am_q)$ are plotted in Figure 4. The data show much larger dependence on the topological charge. A similar dependence is also recently reported in [21]. This result is somewhat unexpected, and probably due to the quenched artifact. In the quenched chiral perturbation theory, the one-loop correction to the pion mass comes from a tadpole diagram with a hairpin insertion. Because of the double pole of singlet pion, the diagram has an infrared divergence in the massless pion limit. Since the hairpin vertex picks up the singlet mass squared m_0^2 , which is proportional to χ_t , the one-loop diagram leads to the quenched chiral logarithm proportional to the global topological charge Q^2 . This is one of the pathologies of quenching.

In order to investigate the topology and volume dependence of the hadron masses, we are planning to carry out simulations at different Q and V .

5. Summary

We reported the current status of our project of dynamical overlap fermion simulation. Although the calculation of the overlap-Dirac operator is so costly, it turned out that its dynamical

simulation is feasible if we fix the global topological charge to suppress the near-zero modes of H_W . In fact, we are able to simulate a $16^3 \times 32$ lattice with quark mass as small as $m_s/6$.

Study of the effects of fixed topological charge is underway. We found that there are local chiral (and thus topological) lumps in the gauge configurations. More study would be necessary to fully understand the effects on physical quantities such as the hadron masses.

Numerical simulations are performed on Hitachi SR11000 and IBM System Blue Gene Solution at High Energy Accelerator Research Organization (KEK) under a support of its Large Scale Simulation Program (No. 06-13). This work is supported in part by the Grant-in-Aid of the Ministry of Education (No. 13135204, 13135213, 15540251, 16740156, 17340066, 17740171, 18034011, 18340075, 18740167).

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