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Twisted-mass reweighting for O(a) improved Wilson fermions

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We test the reweighting of the quark determinant of O(a) improved Wilson fermions in the domain-decomposed hybrid Monte-Carlo algorithm. Specifically, we implement a reweighting in a twisted-mass parameter proposed by Palombi and Lüscher in $N_{\rm f} = 2$ QCD. We find that at equal acceptance rate, the algorithm is significantly more stable on a 32×64^3 lattice upon switching on the reweighting parameter. At the same time, the reweighting factor does not fluctuate strongly and hence is under control. At equal statistics, the uncertainty on the pion correlator is comparable to the case of the standard, unreweighted algorithm.

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1. Introduction

Simulating Wilson type fermions at small quark masses is challenging, in particular because of the potential instabilities caused by the fluctuations of the low modes of the Dirac operator. A direct study of the low-lying spectrum of Wilson Dirac operators reveals that a spectral gap forms for large volume lattices [1]. However, occasional near-zero modes may appear since chiral symmetry is explicitly broken by the discretization. In simulations based on the hybrid Monte-Carlo algorithm (HMC, [2]), this effect can lead to large 'spikes' in the history of the molecular dynamics Hamiltonian violation. Some time ago, Palombi and Lüscher proposed [3] to reweight the fermion determinant so that the zero modes are suppressed by construction. The low-mode contribution to any observable is faithfully restored by including the reweighting factor in the ensemble average. For a review of other applications of reweighting with various fermion discretizations, see the contribution of A. Hasenfratz at this conference.

In the simplest version of the idea, a twisted mass term is added to the Dirac operator,

$$D(\mu) = D_W + i\mu\gamma_5\,, \tag{1.1}$$

where D_W is the $\mathcal{O}(a)$ improved Wilson Dirac operator (see e.g. [4]). For $N_{\rm f} = 2$, the weight

$$W = \det\left(\frac{D_W^\dagger D_W}{D_W^\dagger D_W + \mu^2}\right) \tag{1.2}$$

should be included in the expectation value of the observable $\mathcal{O}$,

$$\langle\mathcal{O}\rangle = \frac{\langle\mathcal{O}W\rangle_\mu}{\langle W\rangle_\mu}\,, \tag{1.3}$$

where $\langle\cdots\rangle_\mu$ stands for the ensemble average for the modified Dirac operator $D(\mu)$.

Evaluating the reweighting factor W exactly is normally not possible, nor is it in fact required; instead it can be calculated stochastically. One may add a set of N pseudo-fermion fields (η_k, $k = 1,\ldots,N$) to the theory with action

$$S_\eta = \sum_{k=1}^{N}(\eta_k,\eta_k)\,, \tag{1.4}$$

and the reweighting factor is replaced by

$$W_N = \frac{1}{N}\sum_{k=1}^{N}\exp\left\{\left(\eta_k,\left[1-\frac{D_W^\dagger D_W+\mu^2}{D_W^\dagger D_W}\right]\eta_k\right)\right\}. \tag{1.5}$$

The simulation with respect to the modified Dirac operator proceeds as before and the reweighting factor W is estimated, for each gauge configuration, according to Eq. (1.5) with N randomly chosen pseudofermion fields. Obviously, the larger the number of pseudofermion fields, the more accurate the estimate. Our tests show that 40 pseudofermion fields are sufficient to yield satisfactory reweighted measurements of meson correlators on $32^3\times 64$ lattices. As is visible from Eq. (1.5), fluctuations in the reweighting factor W that strongly suppress the contribution of certain configurations to the statistical average can occur if the original Dirac operator D_W admits very small eigenvalues.

Convincing arguments were given by Palombi and Lüscher that the reweighting factor would not end up being exponentially small in the volume, as one would at first expect. This follows from the fact that the fluctuations of the lowest eigenvalues become smaller when the volume is increased [1] (possibly with the exception of a few). Nevertheless an explicit test is needed to ascertain that the twisted-mass reweighting idea works in practice, and this is the subject of this work.

2. Implementation

We use the domain decomposition preconditioning [5] of the hybrid Monte-Carlo algorithm (DDHMC). Our simulation code is based on Lüscher's open-source DDHMC code [6]. In this algorithm, the whole lattice is divided into check-board coloured blocks. Using Ω or Ω^* to denote the union of white or black blocks respectively, the Dirac operator assumes the form

$$D_W = \begin{pmatrix} D_\Omega & D_{\partial\Omega} \\ D_{\partial\Omega^*} & D_{\Omega^*} \end{pmatrix}, \tag{2.1}$$

where D_Ω, D_{Ω^*} denotes the Dirac operator respectively on block Ω, Ω^* with Dirichlet boundary condition, and $D_{\partial\Omega}$ is the sum of all hopping terms from the exterior boundary $\partial\Omega$ of Ω to the boundary $\partial\Omega^*$ of Ω^*. The fermion determinant is factorized into local block parts and a global part. For $N_\mathrm{f} = 2$ it reads

$$\det D_W^\dagger D_W = \det R^\dagger R \cdot \prod_\Lambda \det D_\Lambda^\dagger D_\Lambda \,, \tag{2.2}$$

where Λ runs through every block and

$$R = 1 - P_{\partial\Omega^*} D_\Omega^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*}. \tag{2.3}$$

With even-odd preconditioning on every block determinant, Eq. (2.2) can be further written as

$$\det R^\dagger R \cdot \prod_\Lambda \left[\det\left(Q_{ee}^\dagger Q_{ee}\right) \det\left(Q_{oo}^\dagger Q_{oo}\right) \det\left(Q_{ee}^{-1}\widehat{Q}\right)^\dagger \left(Q_{ee}^{-1}\widehat{Q}\right) \right], \tag{2.4}$$

where

$$\widehat{Q} = Q_{ee} - Q_{eo} Q_{oo}^{-1} Q_{oe} \tag{2.5}$$

and the site ordering has been chosen so that D_Λ has the form

$$\gamma_5 D_\Lambda = \begin{pmatrix} Q_{ee} & Q_{eo} \\ Q_{oe} & Q_{oo} \end{pmatrix}. \tag{2.6}$$

The forces of the MD evolution steps are

$$(\omega, F_\Lambda) = 2\mathrm{Re}\left(\widehat{Q}^{-1} Q_{ee}\phi_\Lambda, \delta_\omega\left(\widehat{Q}^{-1} Q_{ee}\right)\phi_\Lambda\right) - 2\mathrm{ReTr}\left(\frac{\delta Q_{ee}}{Q_{ee}} + \frac{\delta Q_{oo}}{Q_{oo}}\right), \tag{2.7}$$

$$(\omega, F_R) = 2\mathrm{Re}\left(R^{-1}\phi_R, \delta R^{-1}\phi_R\right), \tag{2.8}$$

where ϕ_Λ is the pseudofermion fields supported on the even sites of block Λ and ϕ_R is the pseudofermion field residing on the block boundaries.

The modifications required to introduce the twisted mass term are relatively benign. For the modified Dirac operator Eq. (1.1), the fermion determinant becomes

$$\det D(\mu)^\dagger D(\mu) = \det(D_W - i\mu\gamma_5)(D_W + i\mu\gamma_5) \tag{2.9}$$

where the reweighting parameter μ appears with opposite sign for up and down quarks. The forces take the form

$$\begin{aligned}(\omega, F_\Lambda) = 2\mathrm{Re}\left(\widehat{Q}(\mu)^{-1}(Q_{ee}+i\mu)\phi_\Lambda, \delta_\omega\left(\widehat{Q}(\mu)^{-1}(Q_{ee}+i\mu)\right)\phi_\Lambda\right) \\ - 2\mathrm{ReTr}\left(\frac{Q_{ee}\delta Q_{ee}}{Q_{ee}^2+\mu^2} + \frac{Q_{oo}\delta Q_{oo}}{Q_{oo}^2+\mu^2}\right),\end{aligned} \tag{2.10}$$

$$(\omega, F_R) = 2\mathrm{Re}\left(R(\mu)^{-1}\phi_R, \delta_\omega R(\mu)^{-1}\phi_R\right), \tag{2.11}$$

where

$$\widehat{Q}(\mu) = Q_{ee} + i\mu - Q_{eo}(Q_{oo}+i\mu)^{-1}Q_{oe}, \tag{2.12}$$

$$R^{-1}(\mu) = 1 - P_{\partial\Omega^*} D(\mu)^{-1} D_{\partial\Omega^*}. \tag{2.13}$$

Note that to calculate the global force F_R, one needs to solve the full Dirac equation in every integration step. It is therefore important to solve the equation efficiently. The deflation accelerated [7, 8], Schwartz-alternating-procedure (SAP, [9]) preconditioned GCR algorithm is applied. Since the deflation subspace need not be exact, it is constructed by a relaxation process, starting from a set of random quark fields ψ_l, which are updated iteratively according to

$$\psi_l \to \text{“}D_W^{-1}\text{“}\ \psi_l, \tag{2.14}$$

until the condition $||D_W\psi_l|| \leq M\psi_l$ is satisfied, where M is in the range of low eigenvalues of $(D_W^\dagger D_W)^{1/2}$, and “D_W^{-1}“ is an iterative procedure that approximates the inverse of D_W. In the current implementation [6], it is done with the SAP. The operator D_W is used in the relaxation procedure, the deflation efficiency for the operator $D(\mu)$ is equally good, because the deflation subspace needs not to be exact and μ normally is small in practice.

The little Dirac operator, i.e. restriction of the Dirac operator $D(\mu)$ to the deflation subspace, is then specified as matrix

$$A_{kl}(\mu) = (\psi_k, D(\mu)\psi_l). \tag{2.15}$$

The Dirac equation $D(\mu)\psi(x) = \eta(x)$ is separated into two equations by acting with projectors $P_L(\mu)$ and $1 - P_L(\mu)$ from the left, where

$$P_L(\mu)\psi(x) = \psi(x) - \sum_{k,l=1}^{N} D(\mu)\psi_k(x)A(\mu)^{-1}_{kl}(\psi_l, \psi). \tag{2.16}$$

3. Testing

We have tested the reweighting method for two flavors of $\mathcal{O}(a)$ improved Wilson fermions on large lattices ($24^3\times 48$ and $32^3\times 64$) with fine lattice spacings (respectively 0.07 and 0.08 fm). The masses of the lightest pseudoscalar mesons in these ensembles are approximately 360 and 300 MeV

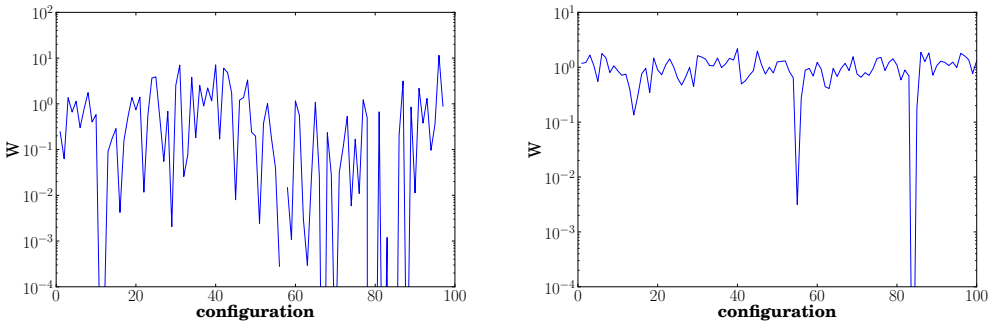

Figure 1: Reweighting factor W on $24^3 \times 48$ lattices for $a\mu = 0.00569$ (left) and 0.003 (right).

respectively. Some details of the simulation, for instance the molecular dynamics trajectory length τ, step size $\delta\tau$, the number of configurations (ncfg) of the generated ensemble and acceptance rate of the HMC simulations are listed in table 1.

The reweighting parameter μ must be chosen with some care. Larger μ accelerates the algorithm but leads to larger fluctuations in the reweighting factor W. We have tested two values of $a\mu$, 0.00569 and 0.003, on $24^3 \times 48$ lattices. The reweighting factors W are calculated according to Eq. (1.5). Their Monte-Carlo history is displayed in Fig. 1, after being renormalized so as to have an average value of one.

For $a\mu = 0.00569$ (left plot), the reweighting factor W fluctuates strongly: about 20% configurations receive a weight that is smaller than 0.01. By contrast, for $a\mu = 0.003$ (right plot), the reweighting factor fluctuates moderately about the mean value. We may use the kurtosis

$$K = \frac{\mu_4}{\sigma^4} - 3\,, \tag{3.1}$$

where μ_4 is the fourth central moment and σ is the standard deviation, to quantify the distribution of the reweighting factor W. For $a\mu = 0.003$, the kurtosis is $K \simeq -0.11$, showing that the fluctuations of W is close to normal distribution; while for $a\mu = 0.00569$, kurtosis rises to $K \simeq 12.8$. Our choice of μ on the $32^3 \times 64$ lattice and the corresponding kurtosis is also listed in table 1.

In our simulations, we have tuned the integration step size of molecular trajectories to achieve an acceptance rate of $\approx 80\%$. For comparison, we have simulated the same set of physical parameters with the standard method ($\mu = 0$), using the same molecular trajectory length. We have tuned the acceptance rate to be similar, $\sim 80\%$. In order to do so, the integration step size had to be roughly 10% smaller. Although both simulations thus ran at similar acceptance rates, we observe that the molecular dynamics trajectories are more stable when reweighting is used compared with

Volume	β	a/fm	m_π/MeV	ncfg	τ	$\delta\tau$	acc. rate	$a\mu$	K
$24^3 \times 48$	5.3	0.07	360	140	0.5	0.028	0.83	0.003	-0.11
$32^3 \times 64$	5.2	0.08	300	120	2	0.013	0.78	0.001	-0.37

Table 1: Parameters of the simulation, as explained in the text. The step size $\delta\tau$ is for updating the global force F_R.

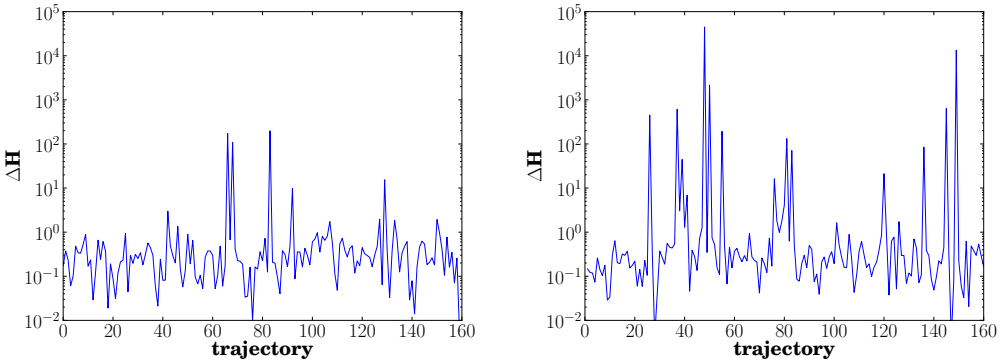

Figure 2: History of Hamiltonian changes of molecular dynamics trajectories in HMC simulations on $32^3 \times 64$ lattices. The reweighting method (left) is more stable than the standard method (right).

the standard method. We plot the changes in Hamiltonian ΔH of molecular dynamics for each trajectory in Fig. 2 for simulations on the $32^3 \times 64$ lattice (reweighting method on the left and standard method on the right). For the reweighting method, the history of ΔH is fairly stable, while for the standard method spikes show up more frequently; the highest spikes are up to three orders of magnitude higher compared to the reweighted algorithm.

Using the reweighting method, we have calculated pion correlators and compared them with the pion correlators measured on the ensembles generated in the standard way. Practically one first measures the correlator in the standard way on the ensemble generated with the reweighting parameter μ; we refer to this correlator as the 'partially quenched' one. Then one 'corrects' it configuration by configuration with the reweighting factor (1.5). In Fig. 3, we plot the partially quenched pion correlator (gray) and the reweighted one (red) and compare them with the pion correlator obtained from the standard simulation (blue). They are compatible within the uncertainties, and have comparable statistical errors.

4. Conclusion

We have implemented a proposal by Palombi and Lüscher to perform a simulation with a quark determinant that is protected from the fluctuations of the low-lying modes. We were able to find a reweighting parameter for which the stability of the DDHMC algorithm is significantly improved, and at the same time the reweighting factor is under control. As a test observable, we found that the correlator of the pseudoscalar density is well behaved under the reweighting (1.3). The behavior of other observables, such as the nucleon correlator, remains to be explored.

In addition to studying the performance of the reweighted algorithm over more than 1000 trajectories, it would be worth trying out other versions of reweighting, where the net benefit in stability is potentially even larger. Palombi and Lüscher for instance made a proposal in this direction [3] in which the UV modes are only affected at order μ^4.

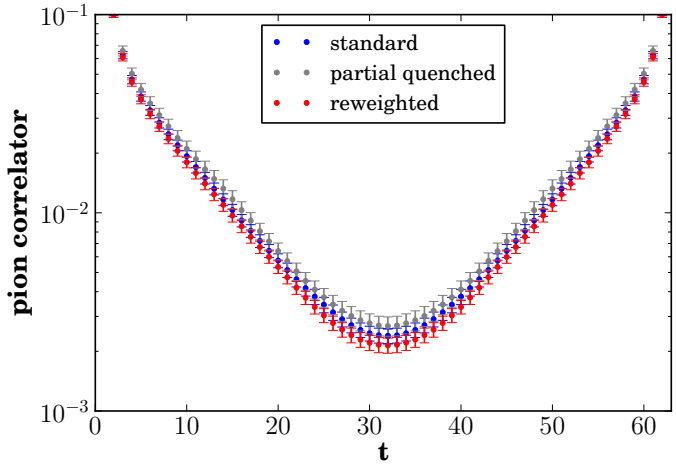

Figure 3: Pion correlator on the $32^3 \times 64$ lattice, with and without reweighting.

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