

Testing Topology Conserving Gauge Actions for Lattice QCD

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We explore gauge actions for lattice QCD, which are constructed such that the occurrence of small plaquette values is strongly suppressed. Such actions originate from the admissibility condition in order to conserve the topological charge. The suppression of small plaquette values is expected to be advantageous for numerical studies in the ε -regime and also for simulations with dynamical quarks. Performing simulations at a lattice spacing of about 0.1 fm, we present numerical results for the static potential, the physical scale r_0 , the stability of the topological charge history, the condition number of the kernel of the overlap operator and the acceptance rate against the step size in local HMC algorithm.

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1. Introduction and motivation

Chiral perturbation theory (χ PT) [1] and lattice QCD are powerful tools to extract quantities at low energy which are relevant for QCD. Lattice QCD simulations can provide the determination of the *Low Energy Constants (LECs)* of χ PT from first principles calculations. A particular situation is found when one enters the ε -regime [2], where

$$m_\pi \sim \frac{1}{L^2} \quad , \quad m_\pi^{-1} > L \quad , \quad \left(L \gg \frac{1}{2F_\pi} \right) . \quad (1.1)$$

There are analytical formulae from χ PT that describe the behaviour of physical quantities in the ε -regime as a function of the volume and the quark mass. These formulae are parametrized by the *infinite volume LECs* of the effective chiral Lagrangian. Therefore we can extract physically relevant information even from the unphysical ε -regime. As a peculiarity of the ε -regime, since one is working in small boxes (1.1 fm \cdots 1.5 fm), observables depend significantly on the topological sector, and predictions exist for expectation values in specific sectors [3]. For the parameters that have been used in the ε -regime simulations, it would be of particular interest to collect large sets of configurations ¹ with the index $|v| > 0$.

In general, however, it is not obvious to define topological sectors on the lattice. A neat definition exists with overlap fermions satisfying the Ginsparg–Wilson relation [5, 6]

$$D_{\text{ov}}^{(0)} \gamma_5 + \gamma_5 D_{\text{ov}}^{(0)} = \frac{1}{\mu} D_{\text{ov}}^{(0)} \gamma_5 D_{\text{ov}}^{(0)} \quad , \quad D_{\text{ov}}^{(0)} = \mu \left[1 + \gamma_5 Q / \sqrt{Q^2} \right] \quad , \quad Q = \gamma_5 (D_{\text{W}} - \mu) \quad , \quad (1.2)$$

where $\mu \gtrsim 1$ is a mass parameter in the operator Q . Since $D_{\text{ov}}^{(0)}$ has exact zero modes with definite chiralities [6, 7, 8], therefore one can use the index as a definition of the topological charge due to the Atiyah–Singer theorem.

While overlap fermions define the fermion-sector of lattice QCD, if one insists on exact lattice chiral symmetry, the lattice gauge action of QCD can be constructed in many ways [9]. One requires the naive continuum limit for all lattice gauge actions to coincide, in which case they fall into the same universality class. The simplest formulation is the *Wilson plaquette action*

$$S_{\text{W}}[U] = \beta \sum_P S_P(U_P) \quad , \quad S_P(U_P) = 1 - \frac{1}{3} \text{Re Tr} U_P \quad , \quad (1.3)$$

where the sum over P runs over all plaquettes.

For the overlap operator (1.2), the topological transitions are excluded under continuous deformations if all the plaquette variables U_P in the configurations involved obey the inequality [10, 11] $S_P(U_P) < \varepsilon = \frac{2}{5d(d-1)} = \frac{1}{30}$ (for all P). Later on H. Neuberger showed a more tolerant bound [12] $\varepsilon = \frac{1}{(1+1/\sqrt{2})d(d-1)} \simeq \frac{1}{20.5}$. For this *admissibility condition*, the exponential locality of the Ginsparg–Wilson fermions is guaranteed [11], and the topological charge is conserved rigorously. However, it is very difficult to realize this condition in the numerical simulation. For practical purposes we have to relax ε to larger values than the analytical bounds.

¹The topologically neutral sector is problematic due to the frequent appearance of very small Dirac eigenvalues, which leads to strong spikes in the Monte Carlo histories of correlation functions [4].

2. Proposal of the gauge actions

We now describe a number of non-standard lattice gauge actions, which suppress the unwanted small plaquette values leading to transitions between different topological sectors. The naive continuum limit of these actions coincides with that of Wilson action (1.3). Based on the proposal by M. Lüscher [10], we consider topology conserving gauge actions [14]

$$S_{\varepsilon,n}^{\text{hyp}}(U_P) = \frac{S_P(U_P)}{[1 - S_P(U_P)/\varepsilon]^n} \quad \text{for } S_P(U_P) < \varepsilon \quad \text{and} \quad +\infty \text{ otherwise,} \quad (2.1)$$

$$S_{\varepsilon,n}^{\text{pow}}(U_P) = S_P(U_P) + \frac{1}{\varepsilon} S_P(U_P)^n, \quad (2.2)$$

$$S_{\varepsilon,n}^{\text{exp}}(U_P) = S_P(U_P) \cdot \exp\{S_P(U_P)^n/\varepsilon\}, \quad (n > 0). \quad (2.3)$$

In simulations, the action (2.1) with $n = 1$ was first used in the Schwinger model [13]. They set $\varepsilon = 1$, i.e. far above the theoretical value of about 0.29, but they still observed topological stability over hundreds of configurations. Here we investigate this type and its extension to the gauge action of lattice QCD.

We show the basic properties of these actions. The left plot of fig. 1 is the histogram of plaquette values for the action $S_{\varepsilon,n=1}^{\text{hyp}}$, compared to the Wilson action, on a 4^4 lattice. In the topology conserving gauge action, the occurrence of very small plaquette values is drastically suppressed. The right plot of fig. 1 shows the ratio of the force in the HMC algorithm between the Wilson plaquette action S_P and topology conserving gauge actions. The action $S_{\varepsilon,n}^{\text{exp}}$ makes a sharp wall *continuous*, but shows the same behaviour as the Wilson action over a wide range.

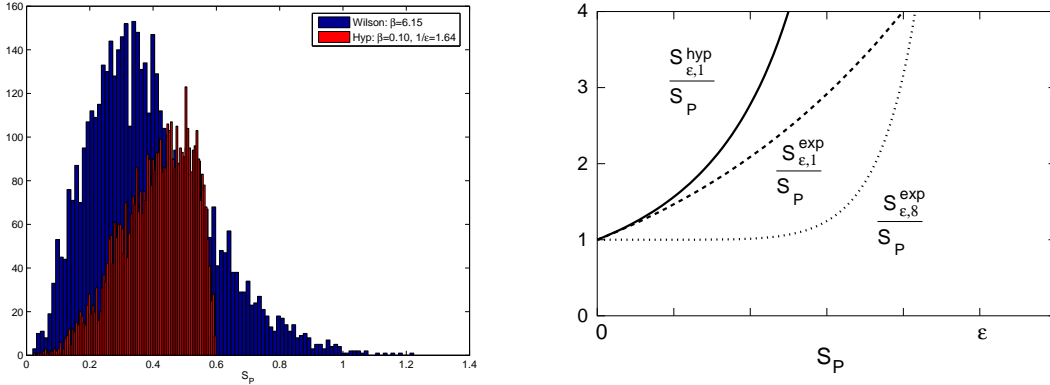


Figure 1: Left: Histograms of S_P for the topology conserving gauge action, compared to the Wilson action, on a 4^4 lattice. Right: Ratio of the force between the Wilson action S_P and modified actions.

For the generation of the configurations we used a *local HMC* algorithm. Since $S_{\varepsilon,n}^{\text{hyp}}$ is non-linear for the link variables, the heatbath and over-relaxation algorithms are not straightforwardly applicable. We use a 16^4 lattice and measure physical quantities every 50 trajectories. See table 1 about the acceptance rate of local HMC. In the value $1/\varepsilon = 1.64$, the acceptance rate is about 65% at the Molecular dynamics step $d\tau = 0.1$. However the acceptance becomes good as $d\tau$ decreases.

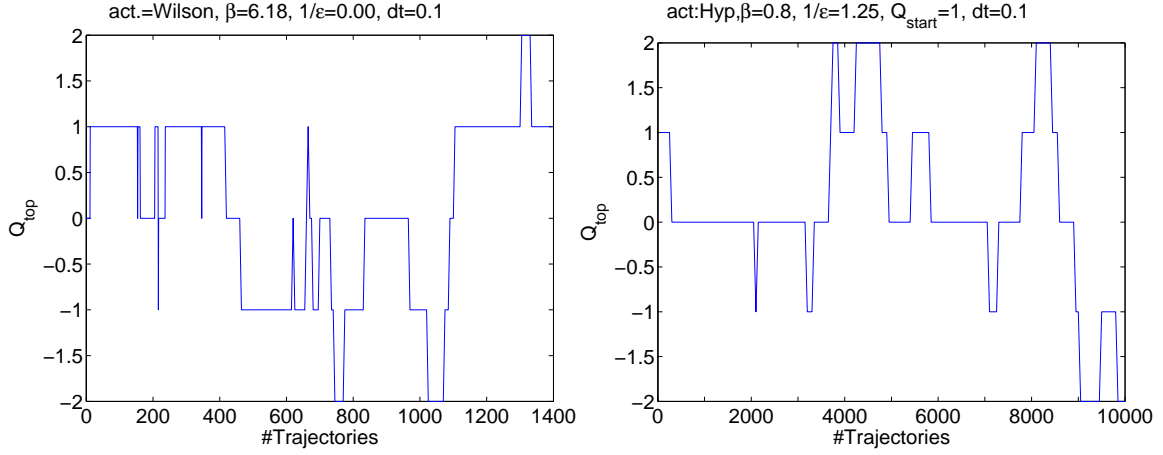


Figure 2: MC-history of Q_{top} for various types of the gauge actions.

3. Monte Carlo history of Q_{top} : Stability of the topological charge.

In fig. 2 we show the Monte Carlo history of the topological charge Q_{top} , which is evaluated by the cooling method², for the Wilson action and the modified gauge actions. The topological charge in $1/\epsilon \ll 20.5$ is not always conserved. However, the changes of Q_{top} are suppressed. Here we define the quantity representing the stability of the topological charge: f_{top} = (the number of jumps of Q_{top}) / (the number of trajectories), see also table 1. The value f_{top} for the modified gauge actions is 10 times smaller than for the Wilson action and thus these actions clearly stabilize the topology charge. Also the autocorrelation of the plaquette τ^{plaq} is getting shorter as $1/\epsilon$ increases. This is important and typical properties of topology conserving gauge actions.

4. The static potential, the physical scale and lattice artifacts

In this section we evaluate the physical scale and the lattice artifacts for various parameters of β and $1/\epsilon$ in the modified gauge actions. The most established method of setting a scale in pure gauge theory is the measurement of the static potential and the force at relatively large distances, extracted from Wilson loops and see *e.g.* Ref. [15].

We show the left plot of fig. 3. A way to check the lattice artifacts [15] is to compare the short distance force at finite lattice spacing with the one extrapolated to the continuum limit $r^2 F(r/r_0)|_c$

$$\Delta(r/r_0) = \frac{r^2 F(r/r_0) - r^2 F(r/r_0)|_c}{r^2 F(r/r_0)|_c}. \quad (4.1)$$

As seen in this figure, for increasing $1/\epsilon$, the discretization errors increase as well. Typically the artifacts of $S_{\epsilon, n=1}^{hyp}$ at $1/\epsilon \gtrsim 1$ are about 10%. Even in $1/\epsilon = 1.64$, the lattice artifact is less than 15%. This is comparable with the Iwasaki and DBW2 gauge actions. Note that the static potential at distance $r \sim r_0$ has not been determined with high precision, and this is reflected in large uncertainties on the quantities $\Delta(r/r_0)$.

²The cooling charges agree in practically all cases with the overlap indices in the range $\mu = 1.3, \dots, 1.6$, as we tested for a subset of the confi gurations.

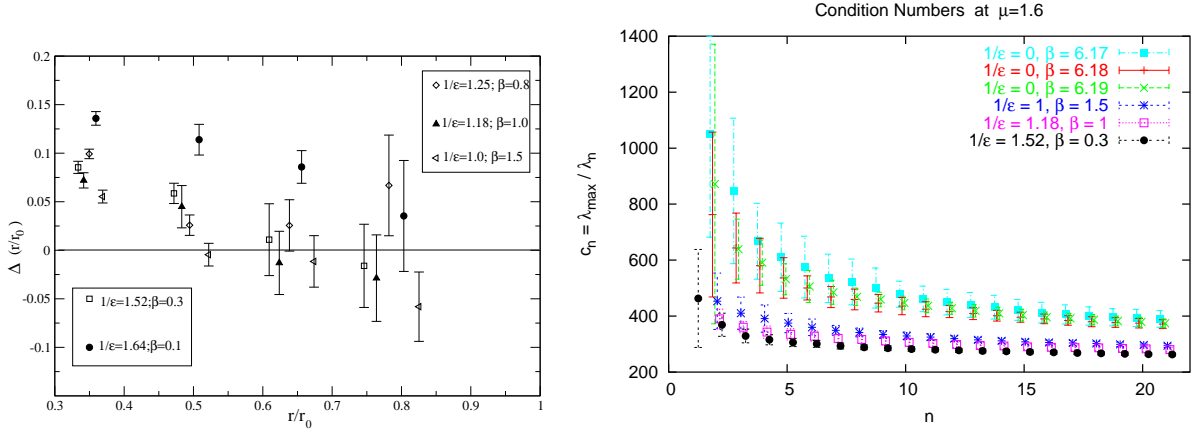


Figure 3: Left: Lattice artifact by the standard estimate for the action $S_{\epsilon, n=1}^{\text{hyp}}$. Right: The conditions numbers $c_2 \dots c_{21}$ at $\mu = 1.6$.

5. Condition number for the overlap operator

We also evaluate the effect of topology conserving gauge actions on the condition number of the overlap operator (1.2). We observe the condition number defined as $C_n = \frac{\lambda_{\max}}{\lambda_n}$ where λ_{\max} is the maximum eigenvalue and λ_n is the n 'th eigenvalue of the kernel Q^2 in the overlap operator. C_n is relevant if $n-1$ modes of Q^2 are projected out. Fig. 3 (right plot) shows the behaviour of the condition number c_2, \dots, c_{21} at $\mu = 1.6$ and about $r_0/a \sim 7.0$. We see an improvement which increases if only a few modes are projected out and if $1/\epsilon$ grows. This means that the numerical computation of $Q/\sqrt{Q^2}$ in the overlap operator gets fast by using topology conserving gauge actions.

6. Summary

Simulations in the ϵ -regime of chiral perturbation theory using the overlap operator can be simplified when appropriate choices of the gauge actions are made. We tested a number of gauge actions that suppress small plaquette values and investigated the properties of these actions [16]. Our results can be summarized as follows, see also table 1.

- The actions of eqs. (2.1, 2.2, 2.3) stabilize the topological charge and could therefore be profitable in QCD simulations in the ϵ -regime.
- The actions of eqs. (2.2, 2.3) are conceptually clean, have a positive transfer matrix and show lattice artifacts that are acceptable and compare well with those of the Iwasaki and DBW2 gauge actions.
- The condition number of the kernel of the overlap operator is improved by using the topology conserving gauge actions when compared to the standard Wilson plaquette action. This speeds up the simulations of overlap fermions in the quenched approximation and will also help in dynamical simulations using the (global) HMC algorithm.

ε^{-1}	β	r_0/a	β_W	$d\tau$	τ^{plaq}	f_{top}	acc. rate
0.	6.19	7.14(3)	6.19	0.1	7(1)	2.2e-2	> 99 %
1.	1.5	6.6(2)	6.13(2)	0.1	2.2(1)	2.4e-3	> 99 %
1.	1.5	6.6(2)	6.13(2)	0.01	2.2(1)	3.2e-3	> 99 %
1.18	1.	7.2(2)	6.18(2)	0.1	1.2(1)	1.6e-3	> 99 %
1.18	1.	7.2(2)	6.18(2)	0.02/0.01	1.3(1)	1.4e-3	> 99 %
1.25	0.8	7.0(1)	6.17(1)	0.1	1.1(1)	2.5e-3	> 99 %
1.52	0.3	7.3(4)	6.19(4)	0.1	0.8(1)	9.4e-4	\approx 95 %
1.64	0.1	6.8(3)	6.15(3)	0.1	1.0(1)	7.0e-4	\approx 65 %
1.64	0.1			0.05	0.7(1)	2.3e-3	\approx 78 %
1.64	0.1			0.025	0.6(1)	3.5e-3	\approx 93 %

Table 1: Results for $S_{\varepsilon,1}^{\text{hyp}}$ for various values of ε and β , on a 16^4 lattice. β_W is the corresponding β of Wilson action to the obtained r_0/a . τ^{plaq} is the autocorrelation time of the plaquette value.

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