Decorrelating Topology with HMC

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The investigation of the decorrelation efficiency of the HMC algorithm with respect to vacuum topology is a prerequisite for trustworthy full QCD simulations, in particular for the computation of topology sensitive quantities. We demonstrate that for \( m_\rho / m_\pi \geq 0.69 \) sufficient tunneling between the topological sectors can be achieved, for two flavours of dynamical Wilson fermions close to the scaling region \( (\beta = 5.6) \). Our results are based on time series of length 5000 trajectories.

1. Introduction

Topology is a fundamental feature of continuum quantum field theories with important bearings on elementary particle physics issues, as there is the proton spin content, the large \( \eta’ \) mass or the role of instantons for the vacuum structure.

Stochastic lattice sampling of QCD configurations must be sufficiently ergodic in the topological sectors of phase space in order to allow for the proper computation of topological quantities. In particular for full QCD, the tunneling rates induced by the hybrid Monte Carlo algorithm between the topological sectors are expected to decrease dramatically when approaching the chiral limit, as known from staggered fermion simulations \[1-3\]. For our investigations, we exploit the SESAM and \( T\chi L \) samples consisting of three time histories on lattices of size \( 16^3 \times 32 \) at \( \kappa = 0.156, 0.157, \) and 0.157, at \( m_\pi / m_\rho \) ratios of 0.839(4), 0.755(7), and 0.69(1), respectively and of configurations on \( 24^3 \times 40 \) lattices, again at \( \beta = 5.6, \) with \( \kappa = 0.1575 \) and 0.158, the latter giving rise to \( m_\pi / m_\rho \approx 0.58(2) \). The length of the samples is 5000 trajectories. For \( \kappa = 0.158 \), the length is 3500 trajectories. From these samples, we take sets of \( N = 200 \) ‘decorrelated’ configurations.

Alternatively, we follow Smit and Vink \[7\] avoiding cooling. With \( G \) being the quark propagator we compute \( Q \) via stochastic estimates \[8\]:

\[
Q(x) = \frac{g^2}{64\pi^2} e^{\mu \nu \rho \sigma} F^\mu \nu(x) F^\rho \sigma(x)
\]

with application of cooling \[9\] as it is not necessary to compute the renormalization of \( Q \).

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In the present investigations, we will just make use of the field theoretical definition \[6\] of the topological charge density

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Q(x) = m \kappa \mathcal{P} \langle \text{Tr}(\gamma_5 G) \rangle_U
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Table 1
First part: mobility \(D_{25}\). Second part: mobility normalized by dividing through square root of the volume.

\[
\begin{array}{cccccc}
\kappa & 0.156 & 0.157 & 0.1575 & 0.1580 & \text{quenched} \\
16^3 \times 32 & 2.8 & 2.5 & 1.9 & - & - \\
24^3 \times 40 & - & - & 3.8 & 2.8 & - \\
16^4 & - & - & - & - & 1.2 \\
\hline
D_{25}/\sqrt{V} & 2.8 & 2.5 & 1.9 & - & - \\
24^3 \times 40 & - & - & 1.9 & 1.4 & - \\
16^4 & - & - & - & - & 1.7 \\
\end{array}
\]

2. Results

In Fig. (1) we present the time series of the topological charge \(Q\) from the five samples. The first three canvases are computed from SESAM ensembles measured on lattices of size \(16^3 \times 32\), the next two are from \(T\chi L\) ensembles from \(24^3 \times 40\) systems. We analyzed every 25th configuration. In the first three graphs, the results from the gluonic and fermionic measurements are superimposed demonstrating nice agreement. For all three SESAM masses, the figure tells us that HMC can create sufficient tunneling in the \(\text{SESAM } m_{\rho}\) window.

We quantify the tunneling between the topological sectors defining the mobility for tunneling as

\[
D_d = \frac{1}{N} \sum_{i=1}^{N} \left| \langle \tilde{Q}(i + 1) \cdot d \rangle - \langle \tilde{Q}(i) \cdot d \rangle \right|.
\]  

(3)

Tab. (1) demonstrates that the mobility is decreasing when going more chiral.

With the \(24^3 \times 40\) system, at \(\kappa = 0.1575\), we can assess the volume dependence. Note that \(Q\) is an extensive quantity. Still we find the tunneling rates sufficient, however, with smaller quark mass, at \(\kappa = 0.158\), the mobility decreases. As we expect the mobility to scale approximately with the square root of the volume, we normalize the numbers accordingly, see the second part of Tab. (1).

Analyzing the time history on every second trajectory (at \(\kappa = 0.1575\)) we find very frequent tunneling, see Fig. (3). On this series, we can compute the autocorrelation function. The exponential autocorrelation time is \(\tau_{exp} = 80(10)\). The integrated autocorrelation time turns out to be \(\tau_{int} = 54(4)\), compatible with the decorrelation of other observables as found in \(\text{[10]}\).
Histogramming Fig. (2) we find a smooth Gaussian, see Fig. (3). This is of course less pronounced for the small decorrelated samples of size 200, see Fig. (3), however, the distributions are still well peaked at $Q = 0$.

3. Summary

As the main result, we find that HMC tunnels well between the vacuum sectors for $\frac{m_\pi}{m_\rho} \geq 0.69$. Autocorrelation times are slightly larger than for the yet worst case observable, the minimal eigenvalue of the Wilson fermion matrix. Therefore, we are confident to be able to carry out reliable computations of hadronic properties related to topology, like the proton spin content and the topological susceptibility for $\frac{m_\pi}{m_\rho}$-values down to 0.69.

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