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Topological susceptibility of SU(3) pure-gauge theory from out-of-equilibrium simulations

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In *JHEP* **04** (2024) 126 [arXiv:2402.06561] we recently proposed an out-of-equilibrium setup to reduce the large auto-correlations of the topological charge in two-dimensional CP^{N-1} models. Our proposal consists of performing open-boundaries simulations at equilibrium, and gradually switching on periodic boundary conditions out-of-equilibrium. Our setup allows to exploit the reduced auto-correlations achieved with open boundaries, avoiding at the same time unphysical boundary effects thanks to a Jarzynski-inspired reweighting-like procedure. We present preliminary results obtained applying this setup to the $4d$ SU(3) pure-gauge theory and we outline a computational strategy to mitigate topological freezing in this theory.

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1. Introduction

Over the last 50 years, lattice field theory has proven to be a successful first-principle approach to the study of the non-perturbative regime of strongly-interacting gauge theories and in particular Quantum Chromo–Dynamics (QCD). Crucial to this success have been the striking advances made in the study and design of algorithms employed to explore their phase space.

Despite these advances, the simulation of theories characterized by topologically non-trivial phase spaces close to the continuum limit remains difficult. This state of affairs is caused by *topological freezing*, a severe divergence of the integrated correlation time τ_{int} of the the topological charge as a function of the correlation length in the approach towards the continuum limit of said theories. In contrast to other cases of critical slowing down for non-topological quantities (e.g., the Wilson loop), where the divergence is polynomial in the lattice correlation length ξ_{L} with a small exponent (typically $\tau_{\text{int}} \sim \xi_{\text{L}}^{z}$ with $z \simeq 2$ in the continuum limit $\xi_{\text{L}} \to \infty$), topological freezing is characterized by a much more dramatic growth. This has been known to affect both SU(N) and Sp($2N$) Yang–Mills gauge theories in four dimensions, as well as other lower-dimensional Quantum Field Theories whose vacuum state possess non-trivial topological features, see Refs. [1–4] and Fig. 1. In practice, this causes the Markov Chain Monte Carlo (MCMC) trajectory of the system to remain trapped in a sector of the phase space with fixed topological charge, and this loss of ergodicity can potentially introduce unwanted biases in the estimation of topological and non-topological physical observables.

Given the theoretical and phenomenological relevance of observables like the topological susceptibility both for QCD hadron phenomenology [5–12] and for Beyond Standard Model physics [4, 13–17], several proposal have been put forward over the years in the attempt of addressing the issue of topological freezing, see Refs. [3, 9, 18–36], and Refs. [37–39] for recent reviews.

A popular strategy in QCD simulations with dynamical fermions consists in performing simulations with Open Boundary Conditions on the temporal side of the lattice [40, 41]. This approach reduces the severity of topological critical slowing down, but at the cost of enhancing finite size effects, which manifest in the form of boundary effects. Another recent strategy that has been extensively applied both in pure-gauge theories [9, 21, 42–48] and in the presence of dynamical fermions [36] combines Periodic and Open Boundary Conditions in a parallel tempering framework (Parallel Tempering on Boundary Conditions—PTBC) in order to avoid systematic boundary effects. In Ref. [49] we have recently proposed a novel approach designed to mitigate topological freezing which shares a few similarities with PTBC. This new setup is rooted on Jarzynski's equality [50] and its application to non-equilibrium evolutions in lattice field theory (see Refs. [51–54]) to combine Open and Periodic Boundary Conditions.

In this contribution, we apply our out-of-equilibrium approach to the four dimensional SU(3) quenched lattice gauge theory. Our aim is to perform a preliminary assessment of the viability of our strategy by measuring the topological susceptibility χ and the integrated autocorrelation time of the topological charge $\tau_{\text{int}}(Q^2)$ at a moderately small value of the lattice spacing. This enables us to perform a comparison with traditional approaches, that are still viable in this regime, and with other recent state-of-the-art algorithms, like the Parallel Tempering on Boundary Conditions. Moreover, this affords us a clear understanding of the computational cost of our approach. This is

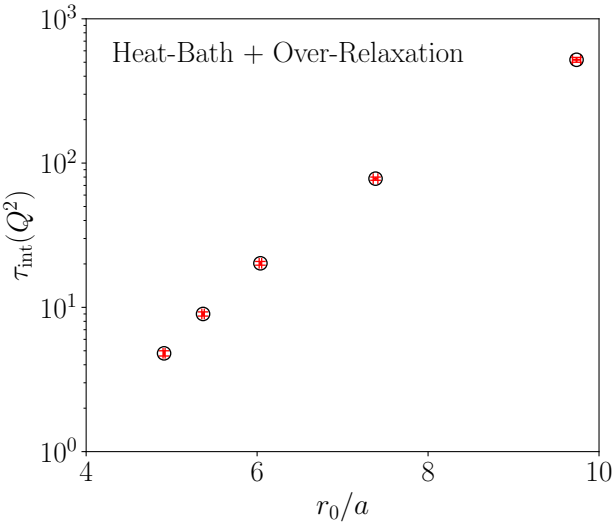

Figure 1: *Growth of the integrated auto-correlation time $\tau_{\rm int}$ of Q^2 as a function of the inverse lattice spacing. This quantity expresses the number of updating steps required to generate two decorrelated measures of Q^2. In this case $\tau_{\rm int}(Q^2)$ is given in units of standard updating steps, defined as 4 lattice sweeps of over-relaxation and 1 lattice sweep of heat-bath. Data for $\tau_{\rm int}(Q^2)$ are taken from dataset generated in Ref. [12], while the scale setting in units of the Sommer parameter $r_0 \simeq 0.5$ fm is taken from the interpolation of the results of Ref. [58].*

the first step towards undertaking the same analysis closer to the continuum limit, where traditional approaches are doomed to fail in sampling non-trivial topology. This also provides a first solid test-bed to implement improvements based on recent machine-learning techniques like Stochastic Normalizing Flows, see for example Refs. [55–57], that fit into this approach quite naturally.

This proceeding is structured as follows. In Sec. 2 we briefly describe our approach and provide details about our setup. In Sec. 3 we report on our numerical results and discuss them. We then conclude and provide a roadmap for the future steps of this analysis in Sec. 4.

2. Setup

Our approach it based on the use of non-equilibrium evolutions and Jarzynski's inequality to resample ensembles of configurations produced with Open Boundary Conditions (on a defect). It is well known that the use of Open Boundary Conditions (OBC) strongly mitigates topological freezing. The crucial difference with Periodic Boundary Conditions (PBC) is the absence, in the former case, of those potential barriers that separate different topological sectors, causing the freezing of topological charge in the first place. While effective in overcoming topological freezing, OBC come with the important drawback of introducing non-physical effects that need to be removed by computing correlation functions sufficiently far from the boundaries. Our strategy is designed to exploit the advantages of OBC without suffering from its pitfalls (similarly to the PTBC algorithm).

First, the so-called defect is defined: a three-dimensional subset of the lattice on which the coupling can be tuned with the purpose of interpolating between OBC, corresponding to coupling 0, to PBC, corresponding to coupling β, like on the rest of the lattice. This is achieved by defining

the system on a hypercubic lattice of length L lattice spacings, with the action

$$S_n[U] = -\frac{\beta}{N_c} \sum_{x,\mu\neq\nu} K^{(n)}_{\mu\nu}(x) \Re \mathrm{Tr} \left[P^{(n)}_{\mu\nu}(x) \right] \tag{1}$$

where $P^{(n)}_{\mu\nu}(x) = U^{(n)}_{\mu}(x) U^{(n)}_{\nu}(x+a\hat{\mu}) U^{(n)\,\dagger}_{\mu}(x+a\hat{\nu}) U^{(n)\,\dagger}_{\nu}(x)$ is the elementary plaquette operator at site x on the plane (μ, ν), and $K^{(n)}_{\mu\nu}(x)$ is a numerical factor used to modify the boundary conditions. It is defined as:

$$K^{(n)}_{\mu\nu}(x) = K^{(n)}_{\mu}(x) K^{(n)}_{\nu}(x+a\hat{\mu}) K^{(n)}_{\mu}(x+a\hat{\nu}) K^{(n)}_{\nu}(x), \tag{2}$$

$$K^{(n)}_{\mu}(x) = \begin{cases} c(n), & \mu = 1, \quad x_1 = L-a, \quad 0 \leq x_0, x_2, x_3 < L_\mathrm{d}, \\ 1, & \text{elsewhere}, \end{cases} \tag{3}$$

where the size of the three-dimensional defect is given by $L_\mathrm{d} \times L_\mathrm{d} \times L_\mathrm{d}$, while $c(n)$ is an *a priori* arbitrary function. The rôle of the latter is to interpolate between OBC when $c = 0$ to PBC when $c = 1$.

Second, an ensemble is obtained from equilibrium MCMC simulation with OBC and the standard combination of local HB+OR updates. We call n_between the number of full lattice sweeps between successive configurations along the Markov Chain with OBC. Each configuration in this ensemble is used as starting point for a non-equilibrium evolution towards a configuration with PBC. In particular, iterations of the same local updating algorithm are run while gradually changing the value of c along a so-called *protocol*,

$$c(n) = 1 - \frac{n}{n_\mathrm{step} - 1} \tag{4}$$

where n_step is the number of steps separating the two different boundary conditions. We remark that in this framework the system does not have to reach equilibrium between successive steps.

Third, any desired observable is calculated on the configurations of the newly obtained ensemble with PBC by performing an appropriate *reweighting* with the statistical weight e^{-W},

$$\langle O \rangle_\mathrm{NE} = \frac{\langle O e^{-W} \rangle_\mathrm{f}}{\langle e^{-W} \rangle_\mathrm{f}}, \tag{5}$$

where W is the *work* spent along a non-equilibrium evolution, that can be calculated explicitly as follows,

$$W = \sum_{n=0}^{n_\mathrm{step}-1} \left\{ S_{n+1}[U_n] - S_n[U_n] \right\} , \tag{6}$$

with U_n the gauge configuration at the n^th step of the out-of-equilibrium transformation.

This strategy behind Eq. (5) can be summarized as follows: we aim at sampling a target distribution p with PBC by reweighting a sample obtained from the prior distribution q_0 with OBC and driven towards PBC through a sequence of non-equilibrium *forward transitions* with probability

$$\mathcal{P}_\mathrm{f}[U_0, \ldots, U] = \prod_{n=1}^{n_\mathrm{step}} \mathcal{P}_n(U_{n-1} \to U_n), \tag{7}$$

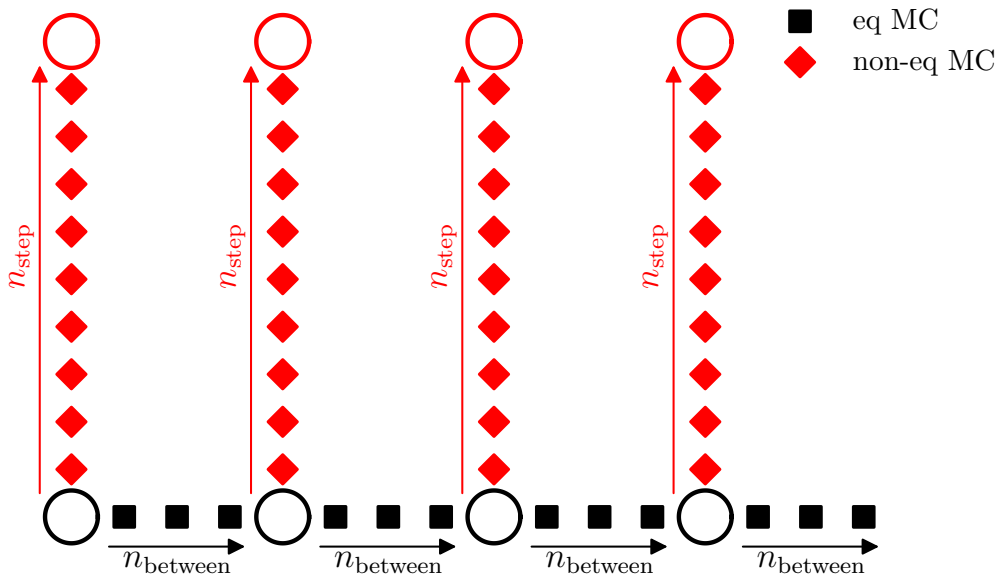

Figure 2: *Sketch of our out-of-equilibrium Monte Carlo setup.*

where each transition probability $\mathcal{P}_n$ is defined by the intermediate action S_n. The expectation value of any observable O with respect to the target distribution

$$p[U] = \frac{1}{Z} e^{-S[U]}, \qquad S \equiv S_{n_{\text{step}}}, \tag{8}$$

can be computed using Eq. (5), where the average over the evolutions is formally defined as

$$\langle \dots \rangle_{\text{f}} = \int [\mathrm{d}U_0 \dots \mathrm{d}U] q_0[U_0] \, \mathcal{P}_{\text{f}}[U_0, \dots, U] \, \dots, \qquad q_0[U_0] = \frac{1}{Z_0} e^{-S_0[U_0]}. \tag{9}$$

We refer to Ref. [49] for a more in-depth discussion of these non-equilibrium evolutions.

A sketch of our out-of-equilibrium Monte Carlo (MC) setup is shown in Fig. 2. The horizontal axis represents equilibrium evolutions with OBCs, used to sample the prior distribution q_0 (OBC). The vertical axis represents out-of-equilibrium evolutions with protocol $c(n)$, used to gradually reach the target distribution p (PBC). The out-of-equilibrium trajectories are n_{step} update steps long, and are separated by n_{between} steps, the latter performed at equilibrium.

The ratio between the partition functions of the prior q_0 and target p, Z_0 and Z respectively, defines the free energy difference ΔF

$$e^{-\Delta F} = \frac{Z}{Z_0}, \tag{10}$$

which can also be computed from the work along the non-equilibrium evolutions using the celebrated Jarzynski's equality [59],

$$\langle \exp(-W) \rangle_{\text{f}} = \exp\left(-\Delta F\right). \tag{11}$$

Of crucial importance is clearly the quality of the sampling of p. This can be evaluated using two figures of merit that estimate how far from equilibrium the evolution is. The first is the reverse

Kullback–Leibler divergence,

$$\widetilde{D}_{\mathrm{KL}}(q_0\mathcal{P}_{\mathrm{f}}\|p\mathcal{P}_{\mathrm{r}}) = \langle W\rangle_{\mathrm{f}} - \Delta F \geq 0, \tag{12}$$

which measures the reversibility of the evolution defined by a given protocol $c(n)$, and the second is the Effective Sample Size (ESS), estimated with

$$\hat{\mathrm{ESS}} \equiv \frac{\langle e^{-W}\rangle_{\mathrm{f}}^2}{\langle e^{-2W}\rangle_{\mathrm{f}}} = \frac{1}{\langle e^{-2(W-\Delta F)}\rangle_{\mathrm{f}}}\,, \tag{13}$$

The ESS has an interesting intuitive interpretation. It is easy to show that the variance of $\langle O\rangle$ obtained from n non-equilibrium measurements is related to the corresponding variance sampled from the target distribution p as follows,

$$\frac{\mathrm{Var}(O)_{\mathrm{NE}}}{n} = \frac{\mathrm{Var}(O)_p}{n\,\mathrm{ESS}}\,. \tag{14}$$

Hence, the former is larger by a factor of $1/\mathrm{ESS}$ with respect to the latter, obtained by sampling p at equilibrium.

In the above formula, the autocorrelations between evolutions have been ignored for simplicity. However, they must be accounted for whenever an estimate of the total cost of using the above strategy is needed. A possible way of estimating the latter was provided in Ref. [49]. We report it here,

$$\mathrm{Var}(O)_{\mathrm{NE}} \times (n_{\mathrm{step}} + n_{\mathrm{between}}) \simeq \mathrm{Var}(O)_p \frac{2\tau_{\mathrm{int}}}{\hat{\mathrm{ESS}}} \times (n_{\mathrm{step}} + n_{\mathrm{between}}). \tag{15}$$

Since this quantity can be computed for any other algorithm, it can be used as a quantitative statistics-independent metric for the efficiency of the algorithm in computing a given observable with a target precision.

3. Numerical results

In this section we report on the preliminary results obtained for the two figures of merit $\hat{\mathrm{ESS}}$ and $\widetilde{D}_{\mathrm{KL}}$ and for the topological susceptibility. All our results refer to simulations conducted for $\beta = 6.40$ on a symmetric $(L/a)^4 = 30^4$ lattice. Assuming $r_0 \simeq 0.5$ fm for the Sommer scale, this point corresponds to a lattice spacing $a/r_0 \simeq 0.1027(5)$, i.e., $a \simeq 0.05$ fm and $L \simeq 1.5$ fm, which is a large enough box to be insensitive to finite-size effects in the topological susceptibility with periodic boundary conditions. The integrated auto-correlation time with PBC of Q^2 was estimated to be $\tau_{\mathrm{int}}(Q^2) \simeq 520(20)$ in units of standard Monte Carlo updating steps using standard algorithms [7], see also the caption of Fig. 1.

The values of the figures of $\hat{\mathrm{ESS}}$ and $\widetilde{D}_{\mathrm{KL}}$ can be calculated as follows. The former is obtained using Eq. (13) on the values of the work defined by Eq. (6). The values of $\widetilde{D}_{\mathrm{KL}}$ are also obtained from the work by direct computation using Eqs. (11) and (12). These quantities were computed for several values of L_{d} and n_{step} and are displayed in Fig. 3 as a function of $n_{\mathrm{step}}/(L_{\mathrm{d}}/a)^3$. In Ref. [49], the latter was identified as the proper scaling variable for these figures of merit in the case of the $2d$ CP^{N-1}. Fig. 3 shows that this is also the case for the $4d$ SU(3) pure lattice gauge theory. Indeed,

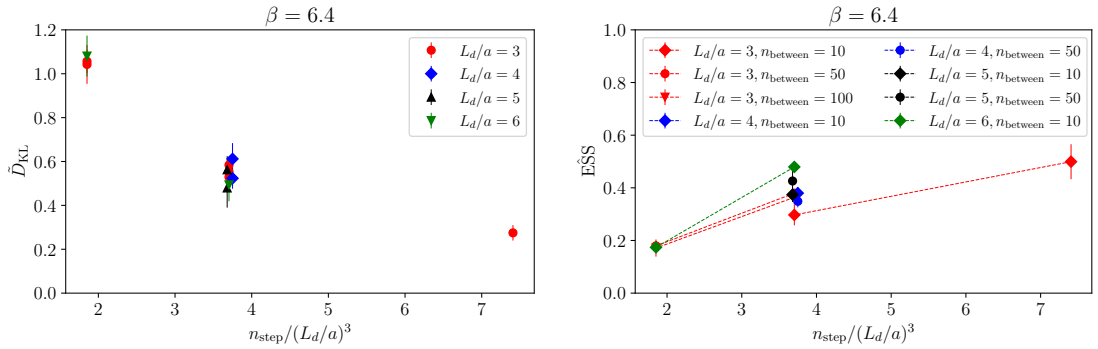

Figure 3: *Figures of merit to quantify how far from equilibrium the evolution is as a function of the length of the out-of-equilibrium trajectory* n_{step} *and of the defect size in lattice units* $(L_{\mathrm{d}}/a)^3$.

to a very good degree of approximation, the values of $\widetilde{D}_{\mathrm{KL}}$ and $\hat{\mathrm{ESS}}$ are seen to collapse on a single curve when represented as a function of $n_{\mathrm{step}}/(L_{\mathrm{d}}/a)^3$. Verifying this scaling is key to understanding how to tune the simulation parameters as the lattice spacing is reduced, and to estimate the cost of a simulation as a function of β.

We now move on to our evaluation of the topological susceptibility. The latter was defined as follows,

$$a^4\chi \equiv \frac{1}{V}\langle Q^2\rangle\,, \tag{16}$$

with $V = (L/a)^4$ and where Q was obtained using a standard clover discretization and computed after 30 cooling steps. We performed several runs with different values of n_{step} and L_{d}. In the left-hand side panel of Fig. 4, we display the non-equilibrium values thus obtained as a function of $\widetilde{D}_{\mathrm{KL}}$. The value of the topological susceptibility obtained with traditional algorithms, see Ref. [12], is represented as a black horizontal line. In all cases, the non-equilibrium and traditional determinations are in agreement within 1.5 standard deviations at most. This shows that, for the values of $\widetilde{D}_{\mathrm{KL}}$ attained in our settings, the susceptibility obtained with non-equilibrium methods is not significantly affected by the details of the simulation and it reproduces the equilibrium estimates.

Finally, in order to assess the efficiency of the non-equilibrium method we have estimated the cost of computing the topological susceptibility with this approach, using the left-hand side of Eq. (15). The latter quantity was computed for each of the available values of n_{step} and L_{d} and is displayed in the right-hand side panel of Fig. 4 as a function of the integrated autocorrelation time $\tau_{\mathrm{int}}(Q^2)$. Smaller autocorrelation times are obtained for larger values of either L_{d} or n_{between}, or both, as expected. In the regime of small autocorrelations, $\tau_{\mathrm{int}}(Q^2) \sim 0.5$–$1.5$, the values of the cost gather around 1, which appears to be the optimal regime for our setup. Given that at the currently explored value of β this was achieved for values of n_{between} and n_{step} of the order of a few hundreds, this means that the cost of 1 decorrelated out-of-equilibrium trajectory in terms of number of updates only improves by a small factor on the results obtained with the standard algorithm, $\tau_{\mathrm{int}}(Q^2) = 520(20)$. However, the gain obtained with our method is expected to increase at larger values of β, owing to the improved scaling of $\tau_{\mathrm{int}}(Q^2)$ obtained with OBC.

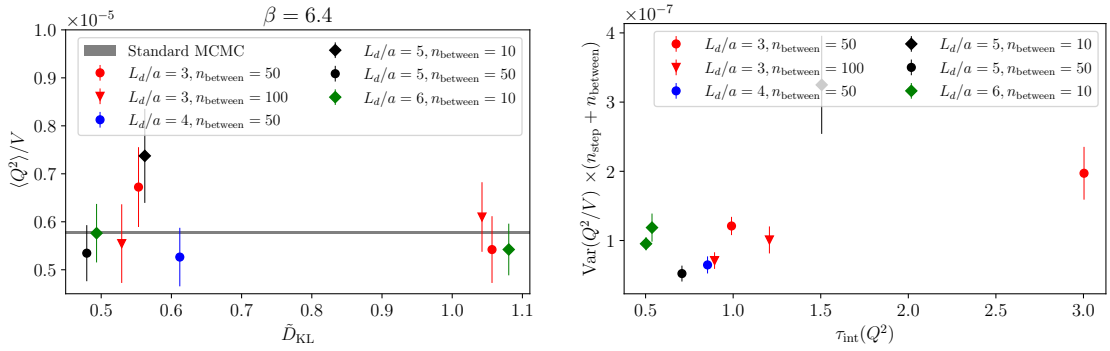

Figure 4: *Left: results for the topological susceptibility. Right: results for the variable defined in Eq.* (15)*, which expresses the efficiency of the out-of-equilibrium algorithm.*

4. Conclusions and future outlooks

In this proceeding we presented a preliminary study of the topological susceptibility of the pure SU(3) lattice gauge theory using out-of-equilibrium simulations. We implemented the same setup already proposed in and tested in Ref. [49], and our results are encouraging. The figures of merit $\hat{\text{ESS}}$ and $\widetilde{D}_{\text{KL}}$ are found to only depend on the scaling variable $n_{\text{step}}/(L_{\text{d}}/a)^3$ rather than on n_{step} and L_{d} separately. Moreover, our estimate of the topological susceptibility is statistically compatible with the estimates present in the literature, with an integrated auto-correlation time for Q^2 that is slightly smaller than the one attained with traditional algorithms.

In the near future we plan to extend the present preliminary study in two different directions. Firstly, by probing larger values of β and by studying systematically how the cost of the out-of-equilibrium behaves as the lattice spacing is reduced. Secondly and most importantly, by combining the setup discussed and described above with the discrete neural network layers composing Normalizing Flows. Stochastic Normalizing Flows fit naturally in the out-of-equilibrium setup, and have the potential of improving the efficiency of our approach even further, see for example the improvement obtained for SU(3) gauge theory in Ref. [57]. This would be achieved by reducing the amount of updating steps necessary to obtain a fixed ESS, at the price of performing a once-and-for-all training procedure with moderate costs.

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