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

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Introduction

Monte Carlo simulations of $4d$ gauge theories with and without fermionic matter are known to be plagued by large auto-correlation times due to slow topological modes on fine lattices.

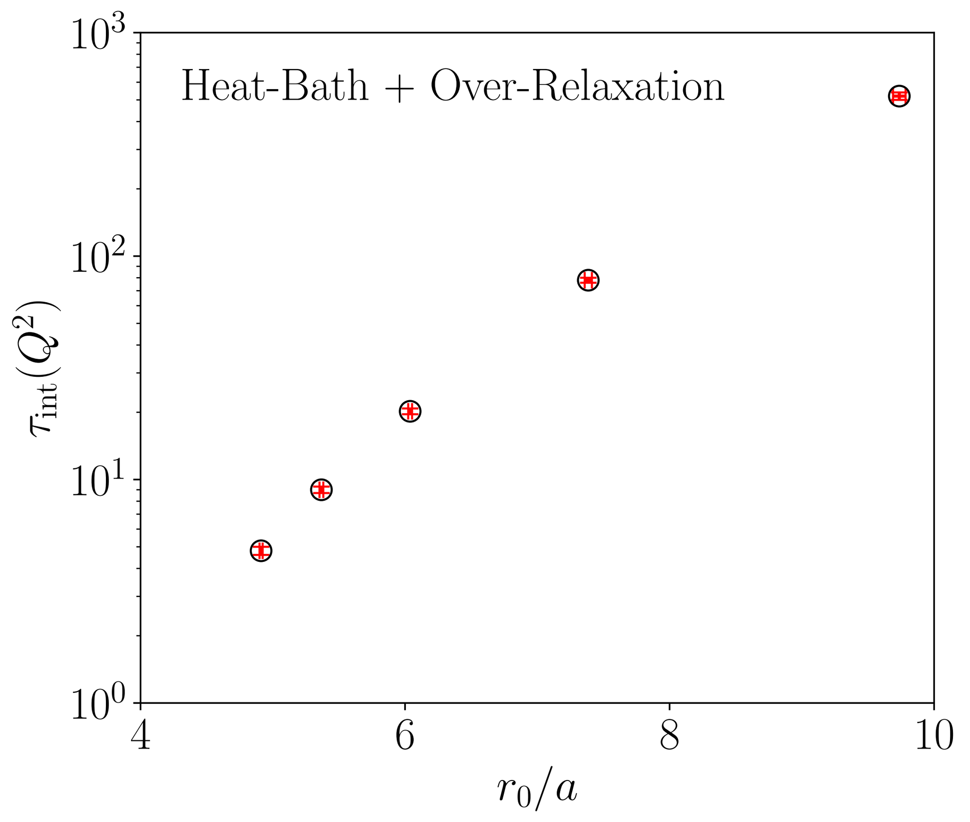
We have recently proposed a novel approach designed to mitigate **topological freezing** that combines a non-equilibrium Monte Carlo with Open Boundary Conditions (OBC).
[Bonanno, Nada, DV, JHEP 04 (2024) 126]
[arXiv:2402.06561]

In this contribution we investigate its application to the case of **4d** SU(3) **Yang–Mills theory**.

Our proposal, already applied to $2d$ CP^{N-1} models, features

- a formal description in terms of non-equilibrium Statistical Mechanics
- a clear understanding of the scaling of the costs with the degrees of freedom
- comparable performances with other recent state-of-the-art algorithms, like Parallel Tempering on Boundary Conditions
- a simple generalization to Stochastic Normalizing Flows

Topological Freezing

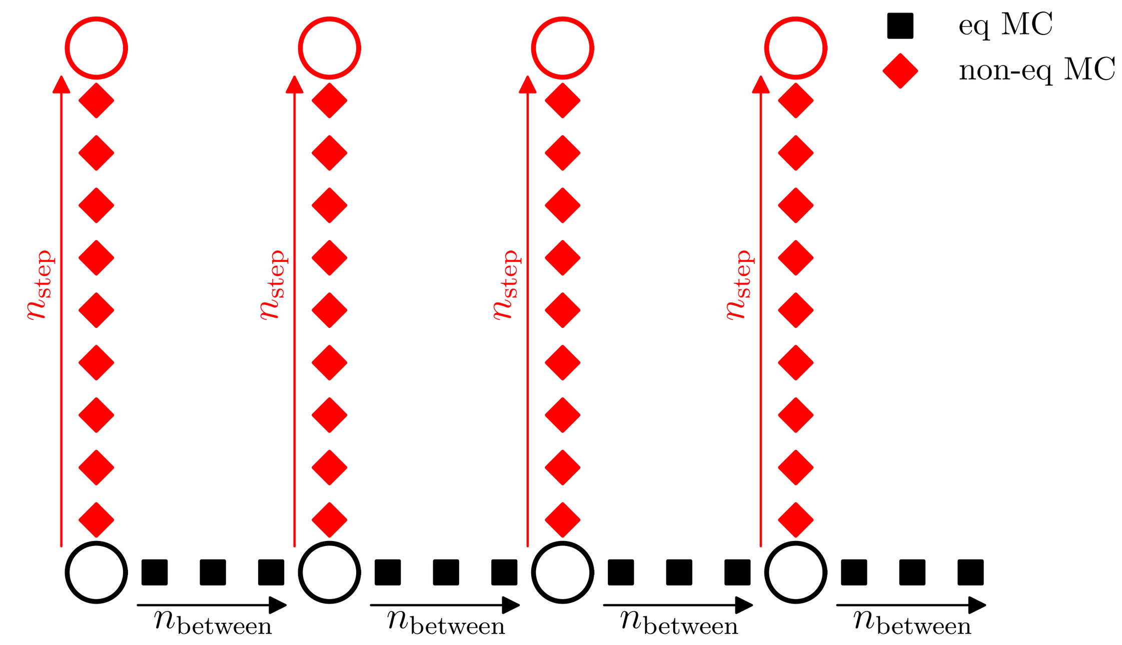


Lattice setup

- Consider a lattice with Periodic Boundary Conditions (PBCs) everywhere but on a small region (**the defect**), subject to Open Boundary Conditions (OBCs).
- Generate a thermalized gauge ensemble with OBCs, separating configurations by n_{between} updating steps
- Starting from OBCs, perform a **non-equilibrium evolution** gradually switching on PBCs
- Links crossing the defect have gauge coupling decreased as $\beta \longrightarrow \beta \times c(n)$ with $0 \le c(n) \le 1$. A linear protocol is used $c(n) = 1 - \frac{n}{n_{\mathrm{step}}-1}$
- Using averages on non-equilibrium evolutions, we obtain expectation values with respect to target distribution (PBCs) starting from prior distribution with OBCs.

$$\chi = \frac{1}{V}\langle Q^2\rangle_{\mathrm{NE}} = \frac{1}{V}\frac{\langle Q^2 e^{-W}\rangle_{\mathrm{f}}}{\langle e^{-W}\rangle_{\mathrm{f}}}$$

Out-of-equilibrium evolutions



Horizontal axis = Equilibrium MC q_0 with OBCs

Vertical axis = Out-of-equilibrium evolution with protocol $c(n)$

Forward transition probability defines the evolution

$$\mathcal{P}_{\mathrm{f}}[U_0,\dots,U] = \prod_{n=1}^{n_{\mathrm{step}}} P_{c(n)}(U_{n-1} \to U_n)$$

Jarzynski's equality is simply

$$\langle \exp(-W)\rangle_{\mathrm{f}} = \exp(-\Delta F)$$

with the work

$$W = \sum_{n=0}^{n_{\mathrm{step}}-1} \left\{ S_{c(n+1)}[U_n] - S_{c(n)}[U_n] \right\}$$

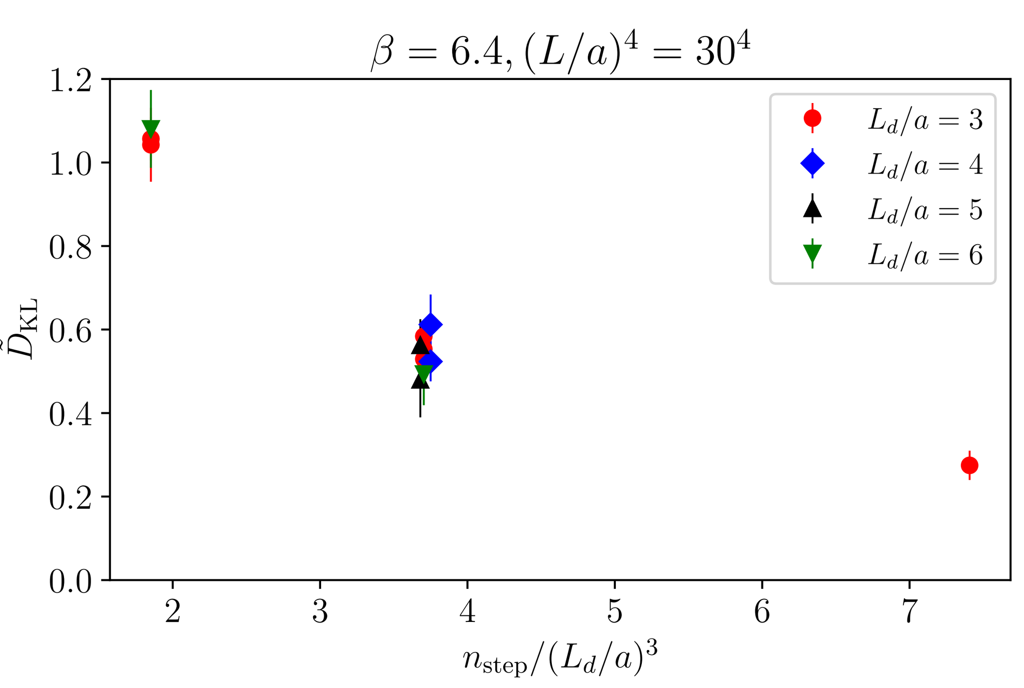
Average over the evolutions is taken as

$$\langle \dots \rangle_{\mathrm{f}} = \int [\mathrm{d}U_0 \dots \mathrm{d}U] q_0(U_0)\, \mathcal{P}_{\mathrm{f}}[U_0,\dots,U] \; \dots$$

The reverse Kullback-Leibler divergence is used to estimate how far from equilibrium the evolution is

$$\tilde{D}_{\mathrm{KL}}(q_0\mathcal{P}_{\mathrm{f}} \| p\mathcal{P}_{\mathrm{r}}) = \langle W\rangle_{\mathrm{f}} - \Delta F \ge 0$$

Scaling with the defect



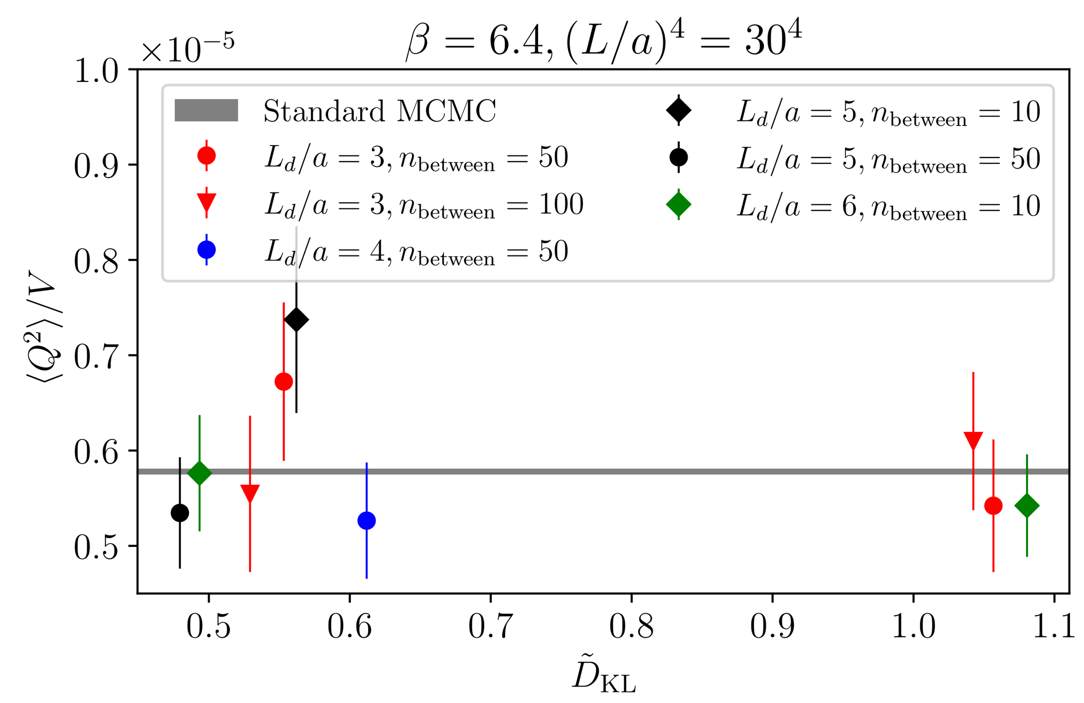
Larger defects imply more degrees of freedom changing along an evolution.

More steps are required for fixed $\tilde{D}_{\mathrm{KL}}$: the scaling is well approximated by

$$n_{\mathrm{step}} \sim (L_d/a)^3$$

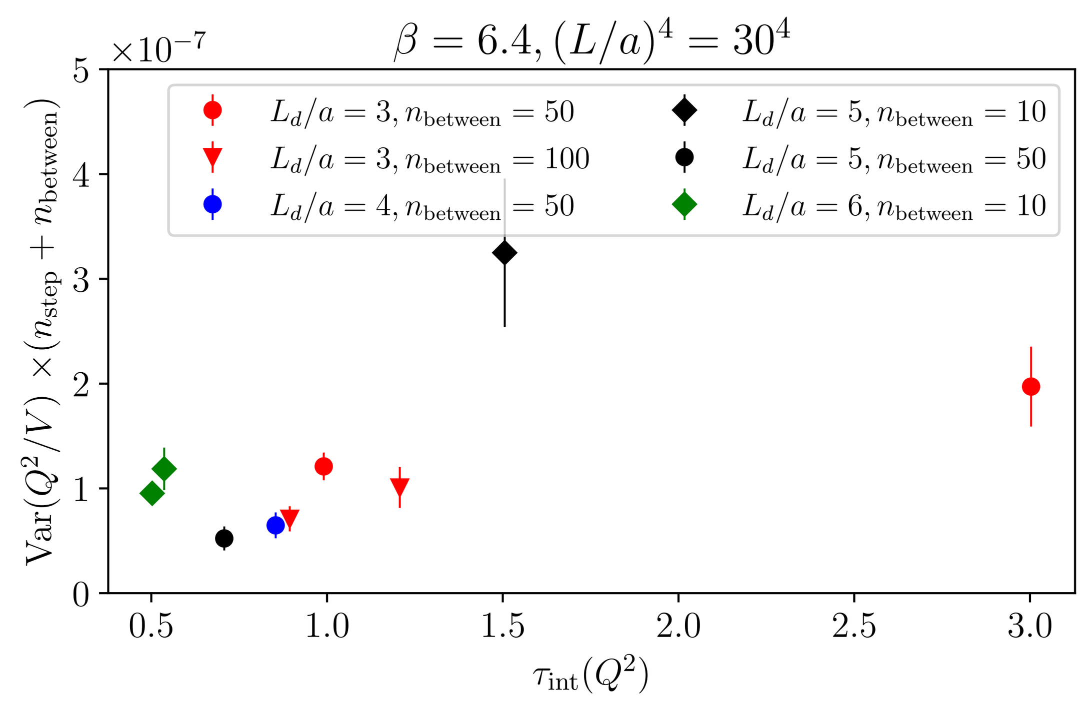
Results for $\beta = 6.40$ on a 30^4 lattice ($a \simeq 0.05$ fm)

To calibrate the algorithm, we tried several combinations of $L_d, n_{\mathrm{step}}, n_{\mathrm{between}}$.



Values for the topological susceptibility are in perfect agreement with results obtained with standard algorithm (PBC).

When sufficiently close to equilibrium the susceptibility is not affected by the details of the evolutions.



Small autocorrelations times are obtained either by using larger L_d or larger n_{between}.

We test the efficiency of the method by looking at the variance of χ times the cost of a single evolution in terms of updates.

Future outlooks

- Perform a systematic investigation of the performances of our out-of-equilibrium setup on even finer lattices
- Extension to Stochastic Normalizing Flows: apply gauge-equivariant layers on the stochastic approach