Metadynamics Surfing on Topology Barriers in the Schwinger Model

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Abstract

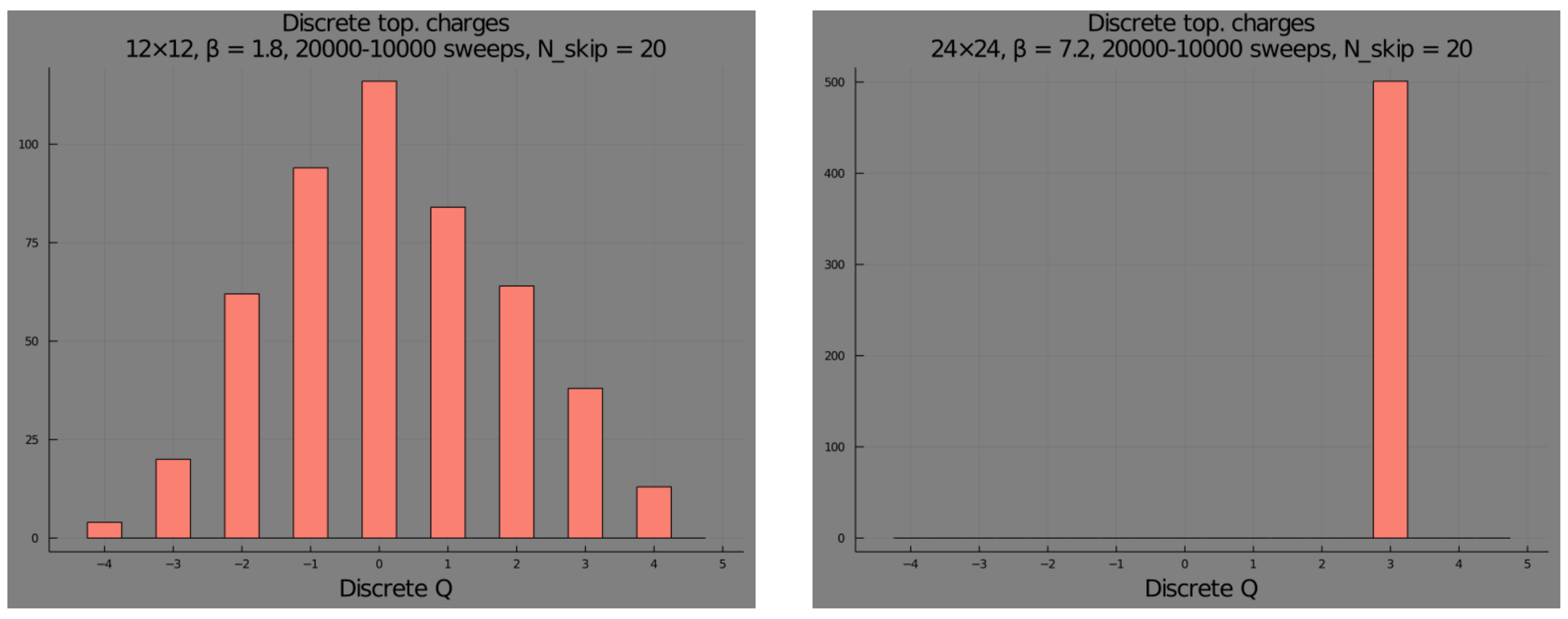
We present our investigation of metadynamics as a solution for topological freezing in 2D U(1) gauge theory. The scaling behavior of the collective variable is examined and a demonstrative measurement of $\langle Q^2 \rangle$ using metadynamics is conducted on finer lattices.

Introduction

Topological freezing describes the increase of the autocorrelation time on increasingly finer lattices when using the Metropolis algorithm. This phenomenon poses an obstacle when approaching the continuum. One observable in the Schwinger model which is particularly prone to topological freezing is the *topological charge* (also *discrete* topological charge)

$$Q = \frac{1}{2\pi} \mathfrak{Im}\Big[\sum_{\vec{n}\in\Lambda} \log P_{xt}(\vec{n})\Big], \tag{1}$$

where $P_{xt}(\vec{n})$ is the plaquette at the lattice site $\vec{n}$. Due to its relatively large autocorrelation time it is well suited to visualize topological freezing:



(a) 12×12-lattice with $\beta = 1.8$ (b) 24×24-lattice with $\beta = 7.2$

Figure 1. Histograms of the discrete topological charge of configurations produced by the Metropolis algorithm on a line of constant physics (LCP) of $N_x N_t / \beta = 80$.

In the Schwinger model *instanton updates* are a possible cure, as they help tunneling to neighboring topological sectors. They involve multiplying a configuration link by link with a (± 1)-instanton configuration, i.e. a local minimum of the gauge action with $Q = \pm 1$. However, the implementation in 4D SU(3) theory remains problematic [1].

Metadynamics

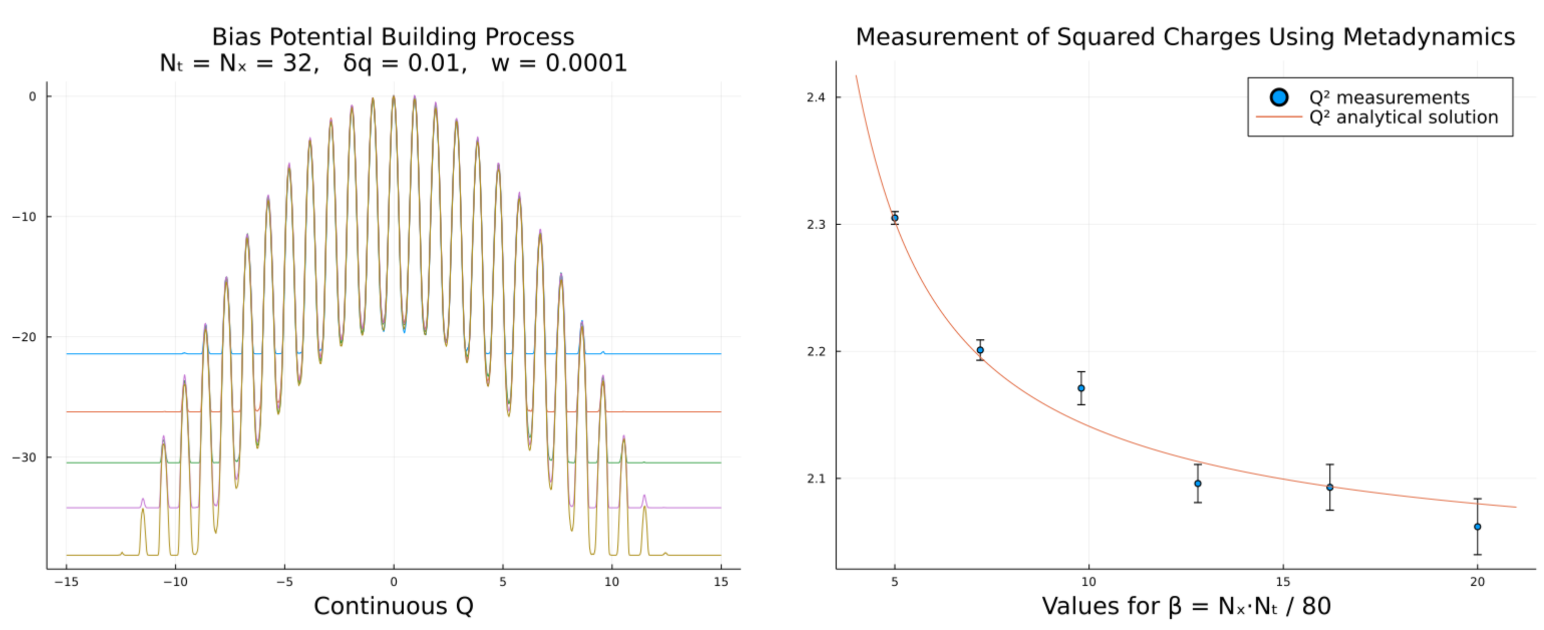
The approach of metadynamics requires to characterize the phase space via *collective variables*. For this Laio et al. [2] suggest using a modified version of the topological charge,

$$Q_{\text{cont}} = \frac{1}{2\pi} \mathfrak{Im}\Big[\sum_{\vec{n}\in\Lambda} P_{xt}(\vec{n})\Big], \tag{2}$$

which we will call *continuous topological charge*, as it is not integer-valued anymore. During a first run one measures Q_{cont} of every configuration x to build up a *metapotential* (also *bias potential*)

$$V(Q_{\text{cont}}(x), t) = \sum_{t'<t} g\Big(Q_{\text{cont}}(x) - Q_{\text{cont}}(x(t'))\Big), \tag{3}$$

which is added onto the gauge action at every Monte Carlo time t. Here $g(Q)$ is a non-negative function that rapidly vanishes for large $|Q|$ (e.g. $w \cdot \exp(-Q^2/2\delta Q)$ with tunable parameters $w, \delta Q$ or small triangles). Figuratively speaking this procedure "fills the local action minima" subsequently until metapotential and gauge action together form a flat overall potential in the region covered.



(a) 32×32-lattice with $\beta = 12.8$ (b) Measurement of $\langle Q^2 \rangle$ for different β

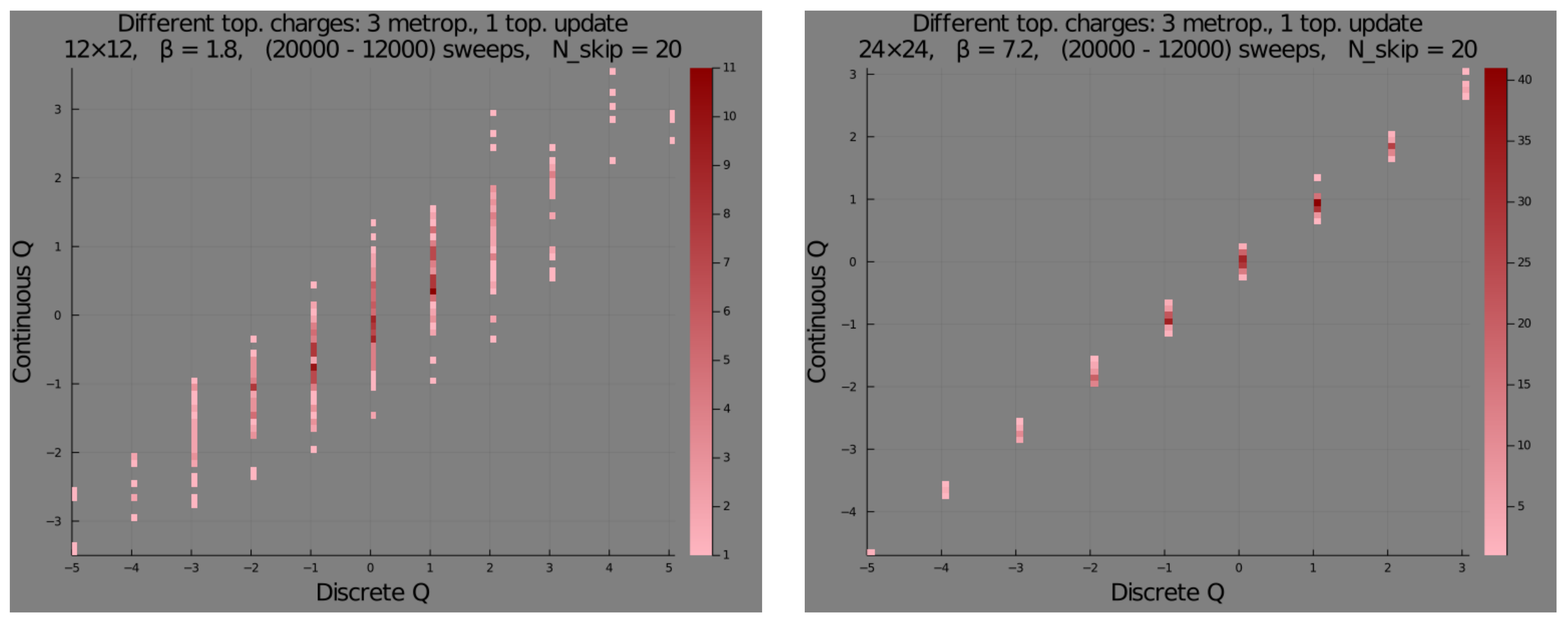
Figure 2. (a) shows snapshots of the metapotential taken at different times during the build up. For comparison the maximum value was subtracted. In (b) measurements of $\langle Q^2 \rangle$ using metadynamics are compared with the analytical prediction [3]. The p-value is $p = 97.8\%$ and $\chi^2/\text{dof} = 7.02/6 = 1.17$.

Once it is built up the metapotential can be added onto the gauge action to obtain a flat potential landscape. Using this in a second run one can measure observables, as the system will not get stuck in topological sectors anymore. This has been done for the observable $\langle Q^2 \rangle$, see Fig. 2(b). Observables will now have to be calculated via reweighting:

$$\langle O \rangle = \frac{\sum_i O_i \exp(-V(Q_{\text{cont},i}))}{\sum_i \exp(-V(Q_{\text{cont},i}))}, \tag{4}$$

Scaling of Q_{cont}

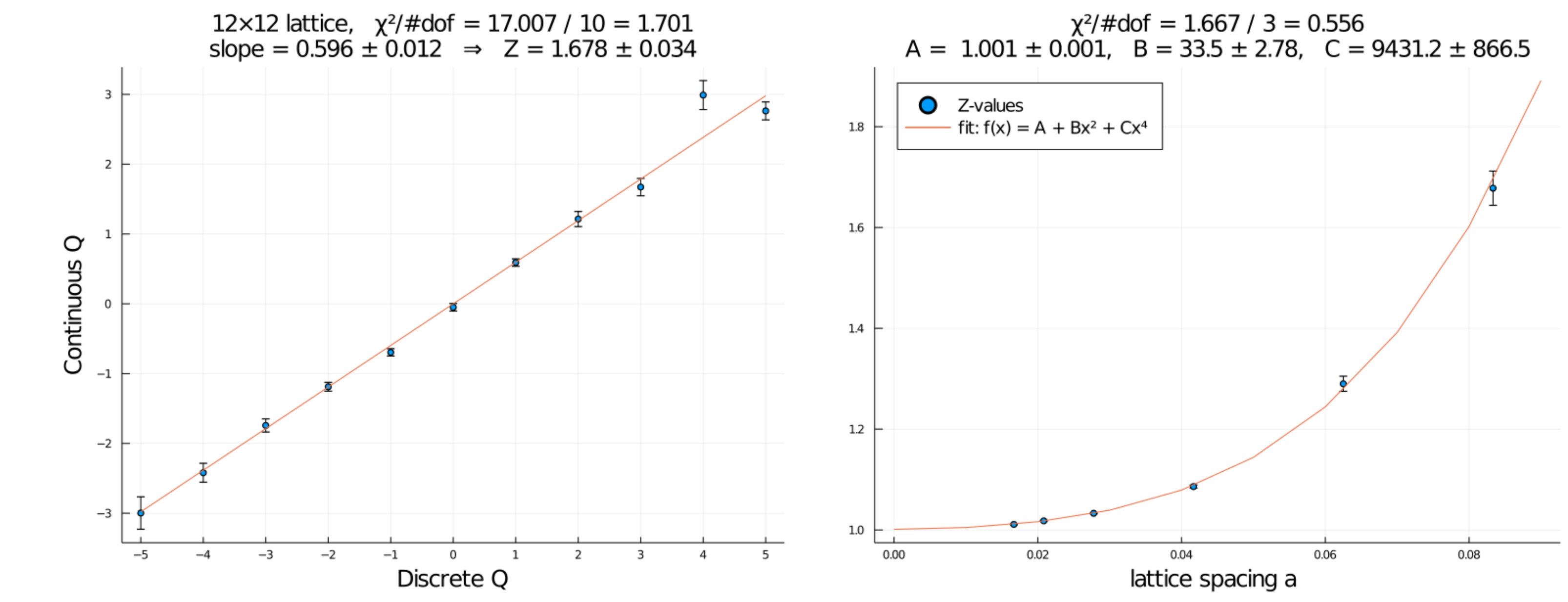
(Q, Q_{cont})-pairs were measured on different lattices of the same LCP:



(a) 12×12-lattice with $\beta = 1.8$ (b) 24×24-lattice with $\beta = 7.2$

Figure 3. 2D histograms of (Q, Q_{cont})-pairs on different lattices of the same LCP.

One can see that the mean values of the Q_{cont}-distributions coincide increasingly better with their respective Q-values for growing lattice sizes. To examine this behavior further, a linear function was fitted to the centers of the Q_{cont}-distributions for each lattice. We called the inverse of the slopes Z and plotted its values against the lattice spacing a, where a is obtained via $\beta = (a^2 g^2)^{-1}$.



(a) Q_{cont}-centers fitted for $\beta = 1.8$ (b) even polynomial fit of Z over a, p-value = 0.64

Figure 4. (a) shows the linear fit corresponding to 3(b). In (b) we see the Z-values for square lattices of $N_t = N_x = 12$ up to $N_t = N_x = 60$ and the best determined fit function, see Eq. (5).

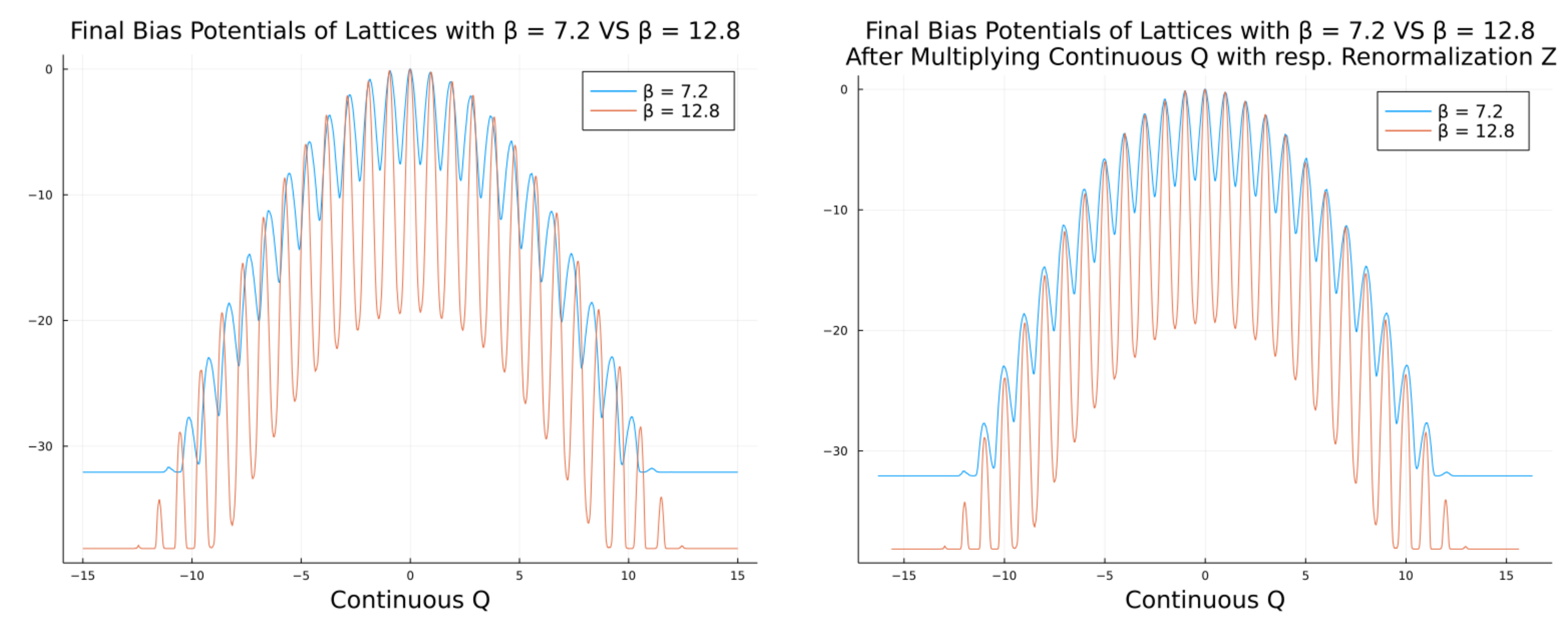
The fitting function describing $Z(a)$ best was determined to be

$$Z_{\text{fit}}(a) = (1.001 \pm 0.001) + (33.50 \pm 2.78)\, a^2 + (9431 \pm 866)\, a^4 \tag{5}$$

and can be seen in Fig. 4(b). An expansion of the topological charge reveals why an even polynomial fit is expected to be the best candidate:

$$Q = Q_{\text{cont}} + c_3\, a^3 + c_5\, a^5 + \ldots \tag{6}$$

Using Eq. (5) we can compare metapotentials of different lattice sizes:



(a) Without multiplying with Z (b) With multiplying with Z

Figure 5. Due to the scaling of the continuous charge one cannot directly compare metapotentials of different β's of the same LCP: one has to multiply the Q_{cont}-values with their respective Z-factors.

Outlook

To counter the drawback of the building time it looks auspicious to explore options of guessing the shape of the metapotential rather than measuring it. For this one might explore the scaling of other quantities such as the barrier height as well, while a fit of the form $F(Q) = AQ^2 + B \sin^2(\pi Q)$ as in [2] seems sensible as well. More generally extracting different modes of the Markov chain would be interesting and could potentially be helpful in constructing better collective variables.
Furthermore one might also implement more general variations, e.g. by using more than one collective variable or well-tempered metadynamics [4], where $g(Q)$ from Eq. (3) has an explicit time dependence.
Last but far from least a comparison to other topology changing algorithms is much-needed, while also a generalization to 4D SU(3) could be very interesting for simulations in QCD. For this we strongly recommend a look at [1]!

References

[1] T. Eichhorn, C. Hoelbling, [arXiv:2112.05188 [hep-lat]]
[2] A. Laio, G. Martinelli and F. Sanfilippo, [arXiv:1508.07270 [hep-lat]]
[3] S. Elser, [arXiv:hep-lat/0103035 [hep-lat]]
[4] A. Barducci, G. Bussi and M. Parrinello, arXiv:0803.3861v1

* Corresponding talk on Mon 08.08. 5:30 PM in HS7 (CP1-HSZ)