

Topology changing update algorithms for $SU(3)$ gauge theory



Timo Eichhorn

Christian Hölbling Philip Rouenhoff Lukas Varnhorst

Bergische Universität Wuppertal

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Introduction

Continuation of [2112.05188] $2D \text{ U}(1) \rightarrow 4D \text{ SU}(3)$



Comparison of topology changing update algorithms

Timo Eichhorn* and Christian Hoerhling

Department of Physics, University of Wuppertal, Gausstrasse 20, D-42119 Wuppertal, Germany
E-mail: timo.eichhorn@uni-wuppertal.de, hoerhling@uni-wuppertal.de

In modern lattice simulations, conventional update algorithms do not allow the tunnelling between topological sectors at low lattice spacing. We compare the stability of multiple free-fermion world-algorithms (metadynamics, insertion updates, and multicanonical formalisms) with respect to proper sampling of all topological sectors in the Schrödinger model. We briefly comment on the prospects of applying these methods to 4-dimensional SU(3) simulations.

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Zinn-Gelehrter-Mathematisches Institut der Universität

*Speaker

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Related talks:

- Parallel tempering:
[talk by Ruben Kara]
- Tempered boundaries:
[talk by Claudio Bonanno]
- Multicanonical:
[talk by Francesco D'Angelo]
- Many more in this session:
[Algorithms I]
[Algorithms II]
[Algorithms III]
[Algorithms IV]

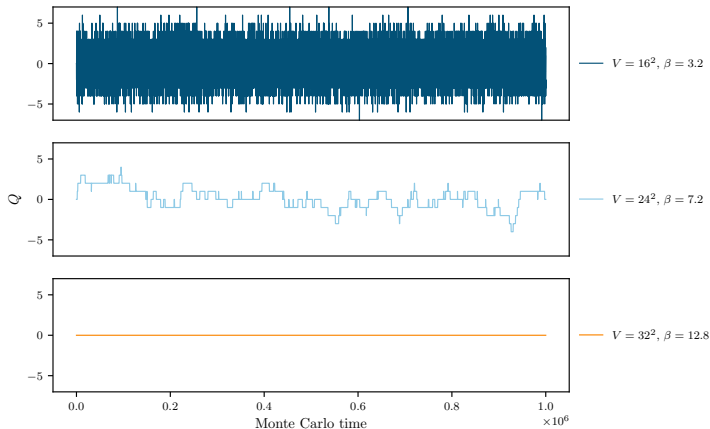
Also see [poster by Philip Rouenhoff]



MOTIVATION

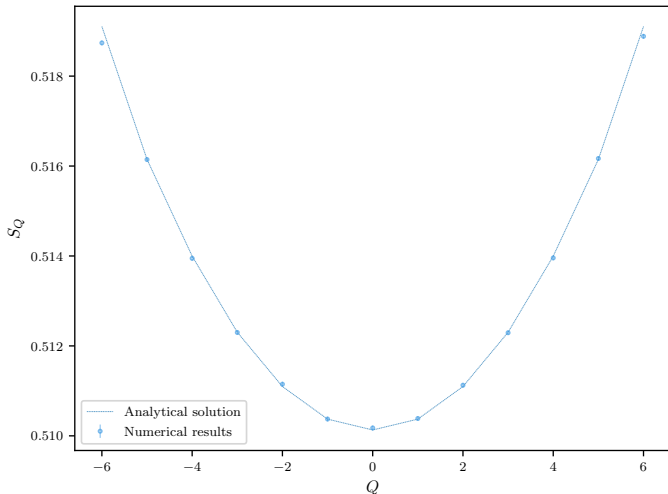
Topological freezing in 2-dimensional U(1)

Not exclusive to QCD/SU(3) gauge theory

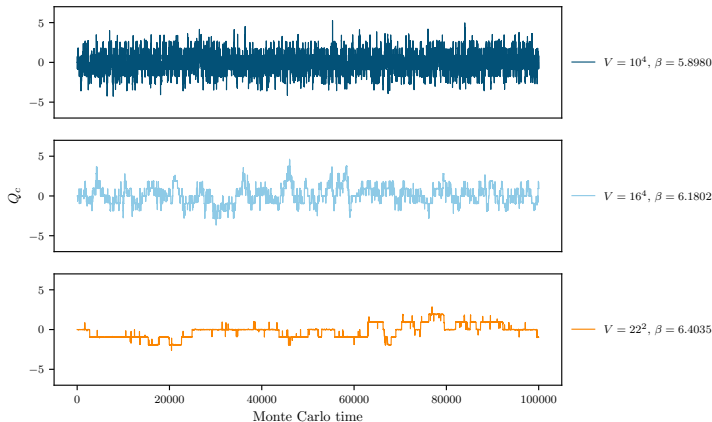


Topological freezing - Consequences

Slow topological modes couple to other observables!



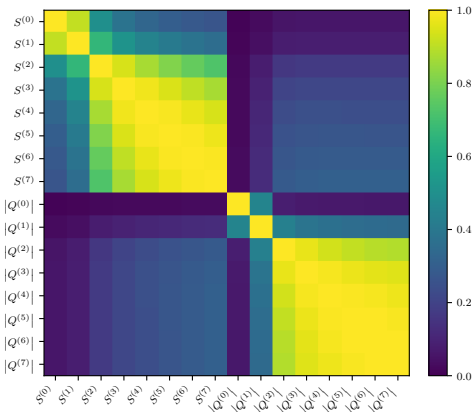
Topological freezing in 4-dimensional SU(3)



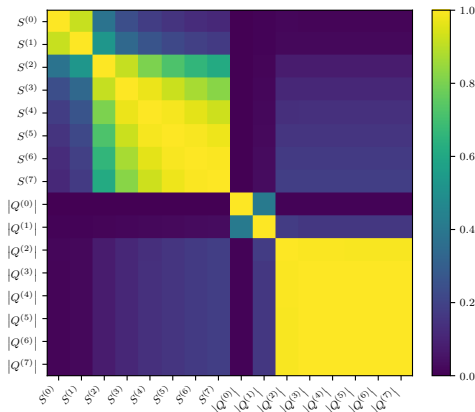
Not yet completely frozen for the lattice spacings considered here

Topological freezing - Consequences

$$V = 10^4, \beta = 5.8980$$



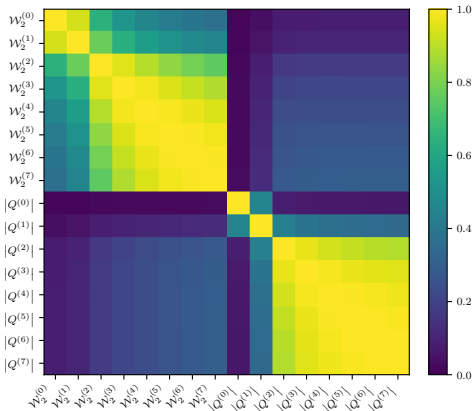
$$V = 22^4, \beta = 6.4035$$



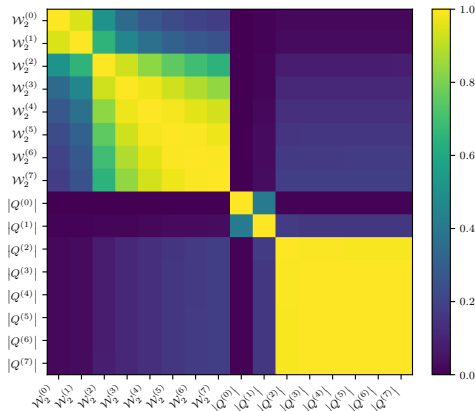
Weak but non-vanishing correlation between action and topological charge!

Topological freezing - Consequences

$$V = 10^4, \beta = 5.8980$$



$$V = 22^4, \beta = 6.4035$$

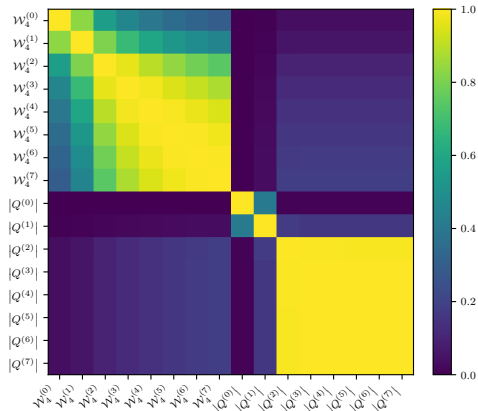
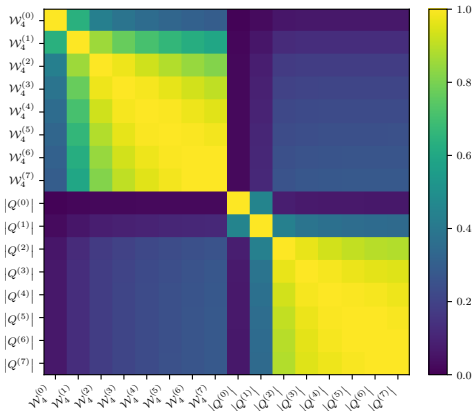


The same can be seen for Wilson loops ($L = 2$)

Topological freezing - Consequences

$$V = 10^4, \beta = 5.8980$$

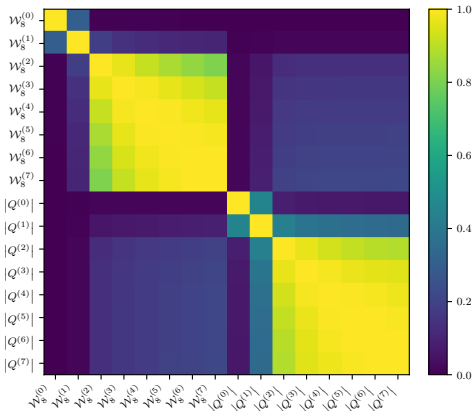
$$V = 22^4, \beta = 6.4035$$



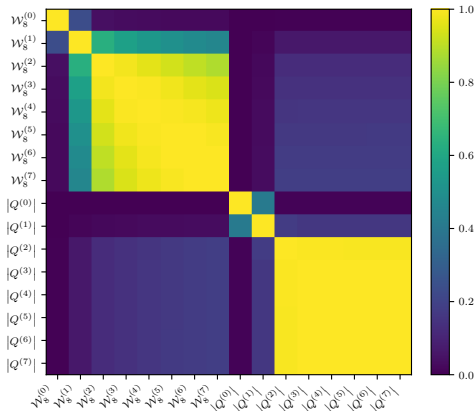
The same can be seen for Wilson loops ($L = 4$)

Topological freezing - Consequences

$$V = 10^4, \beta = 5.8980$$



$$V = 22^4, \beta = 6.4035$$



The same can be seen for Wilson loops ($L = 8$)



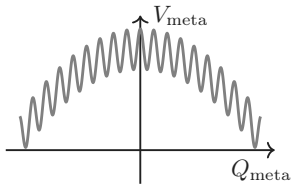
UPDATE ALGORITHMS

Two approaches

Metadynamics

[Laio et al '16]

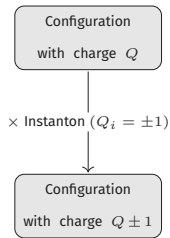
Add history-dependent bias potential to action



Instanton updates

[Fucito et al '84]

Multiply configurations with instantons

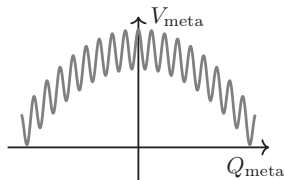


Metadynamics

Metadynamics

[Laio et al '16]

Add history-dependent
bias potential to action



- Requires non-integer definition of Q :

$$Q_c = \frac{1}{32\pi^2} \sum_n \text{tr}[\epsilon_{\mu\nu\rho\sigma} C_{\mu\nu}(n) C_{\rho\sigma}(n)]$$

Here: Clover-definition with under-smeared fields

- After every accepted update, also update V_{meta}
- Add bias potential to action

$$S_{\text{meta}} = S_g + V_{\text{meta}}$$

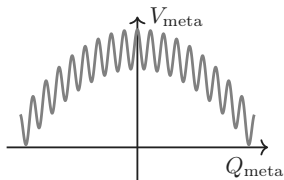
- Reweight observables back to desired distribution

Metadynamics

Metadynamics

[Laio et al '16]

Add history-dependent bias potential to action



- Local update algorithms not feasible:
 - **Heatbath + Overrelaxation:**
No force induced by Metadynamics, doesn't help with tunneling
 - **Metropolis:**
Either compute ΔQ_{meta} for every link update (too expensive) or after one sweep (low acceptance rate)
- Use global updates (**Hybrid Monte Carlo**):
⇒ Force given by sum of normal thin-link force and (fat-link) metadynamics-force:

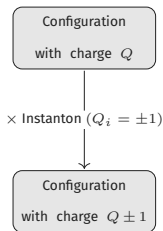
$$\frac{\partial V_{\text{meta}}}{\partial Q_{\text{meta}}} \frac{\partial Q_{\text{meta}}}{U^{(n)}} \star \underbrace{\frac{\partial U^{(n)}}{\partial U^{(n-1)}} \cdots \frac{\partial U^{(1)}}{\partial U}}_{\text{Stout force recursion}}$$

Instanton updates

Instanton updates

[Fucito et al '84]

Multiply configurations
with instantons



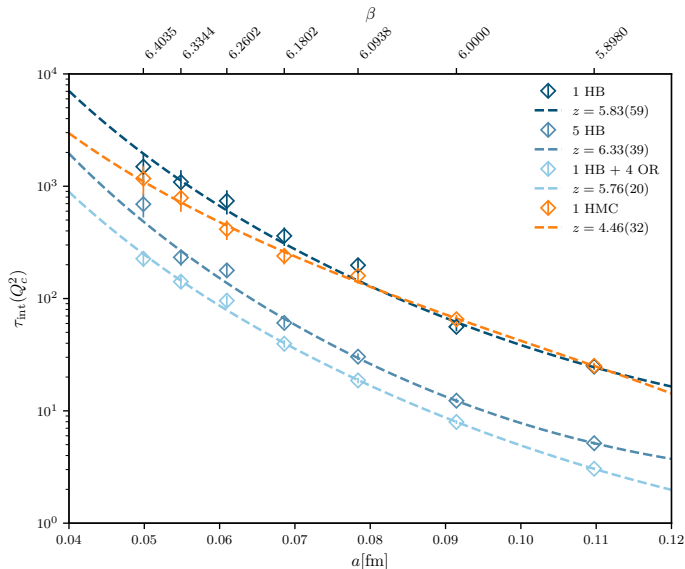
- Link-wise multiplication of initial configuration with $Q_i = 1$ or $Q_i = -1$ instanton
- Add Metropolis accept-reject step
- Works well in Schwinger model
⇒ Advantage: No need to pass through phase space regions with high action



RESULTS

CONVENTIONAL UPDATES

Conventional update algorithms



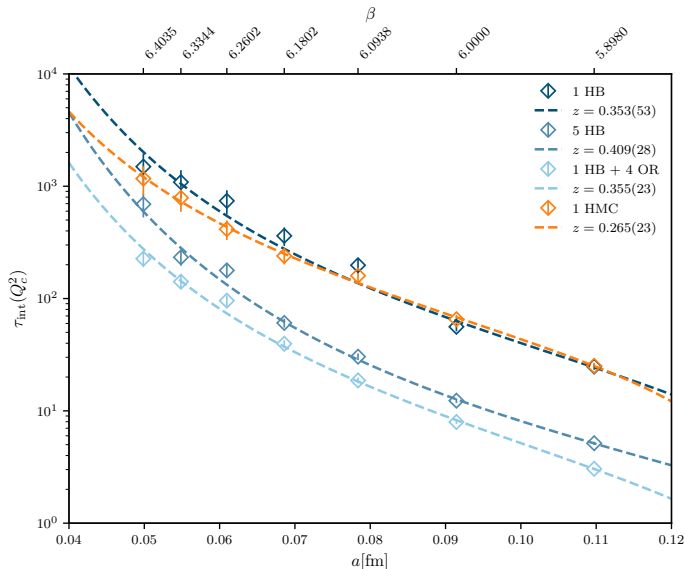
- **HB:** Heatbath over 3 SU(2) subgroups
- **OR:** Overrelaxation over 3 SU(2) subgroups
- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

Topological charge

$$\tau_{\text{int}}(Q_c^2) \propto a^{-z}$$

$$z \approx 5 - 6?$$

Conventional update algorithms



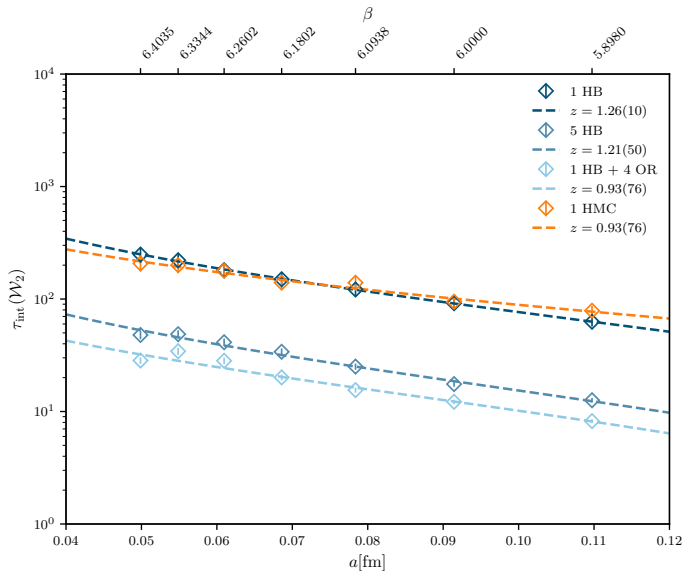
- **HB:** Heatbath over 3 SU(2) subgroups
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- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

Topological charge

$$\tau_{\text{int}}(Q_c^2) \propto e^{\frac{z}{a}}$$

$$z \approx 0.2 - 0.4?$$

Conventional update algorithms



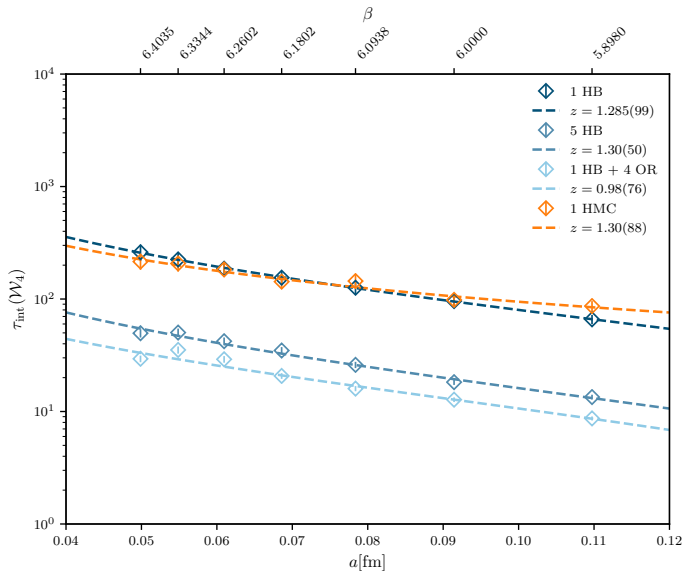
- **HB:** Heatbath over 3 SU(2) subgroups
- **OR:** Overrelaxation over 3 SU(2) subgroups
- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

Smeared Wilson loops

$$\tau_{\text{int}}(\mathcal{W}_2) \propto a^{-z}$$

$$z \approx 1 - 2?$$

Conventional update algorithms



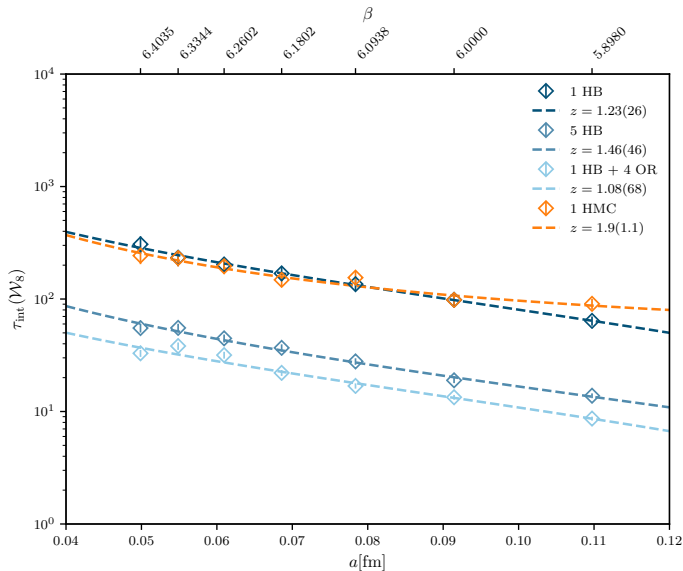
- **HB:** Heatbath over 3 SU(2) subgroups
- **OR:** Overrelaxation over 3 SU(2) subgroups
- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

Smeared Wilson loops

$$\tau_{\text{int}}(\mathcal{W}_4) \propto a^{-z}$$

$$z \approx 1 - 2?$$

Conventional update algorithms



- **HB:** Heatbath over 3 SU(2) subgroups
- **OR:** Overrelaxation over 3 SU(2) subgroups
- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

Smeared Wilson loops

$$\tau_{\text{int}}(\mathcal{W}_8) \propto a^{-z}$$

$$z \approx 1 - 2?$$

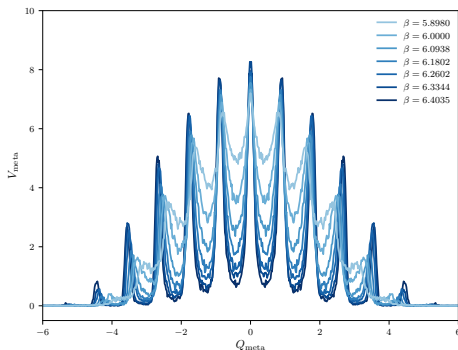


RESULTS

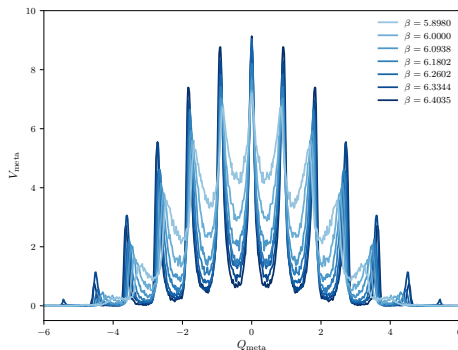
METADYNAMICS

Scaling of metapotential

8 stout



10 stout

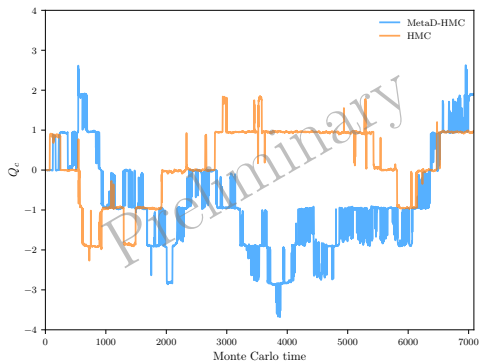


⇒ Smoother potentials (well-tempered Metadynamics or filter?)

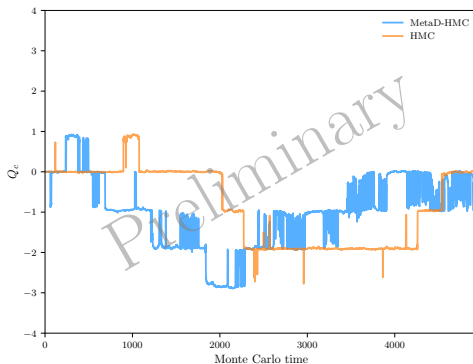
⇒ Tune smearing steps

Metadynamics timeseries

$$V = 18^4, \beta = 6.2602$$

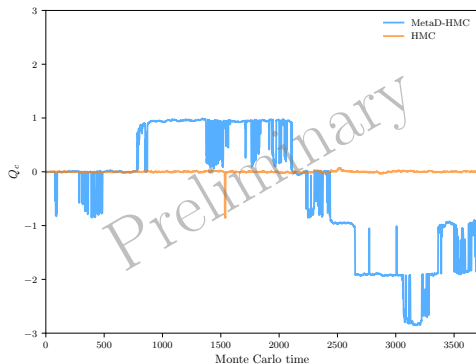


$$V = 20^4, \beta = 6.3344$$



Metadynamics timeseries

$$V = 22^4, \beta = 6.4035$$



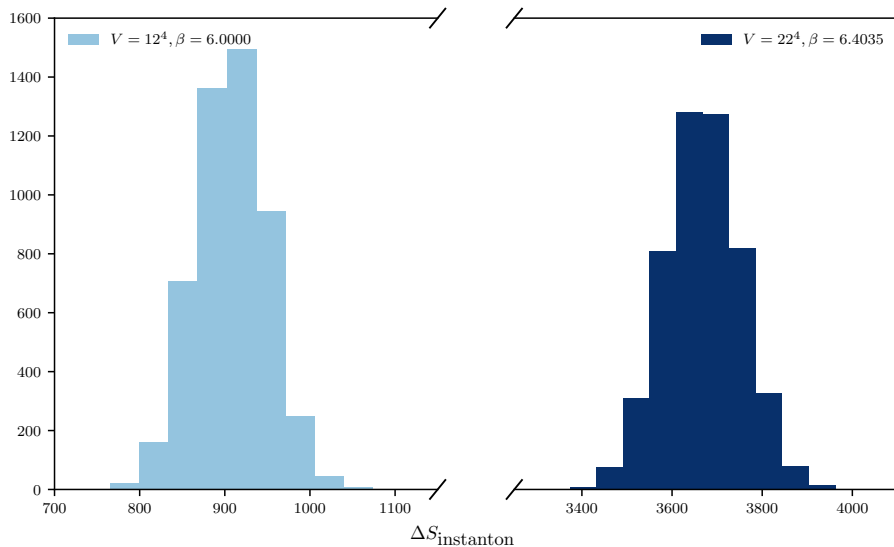
- Modest improvement compared to HMC
- Fluctuations between sectors (suboptimal parameters?)
- Lower acceptance rates
HMC 99% \rightarrow 80% MetaD-HMC
- Much higher computational cost (\sim 20 times slower than HMC!)
 \Rightarrow Not that relevant for full QCD



RESULTS

INSTANTON UPDATES

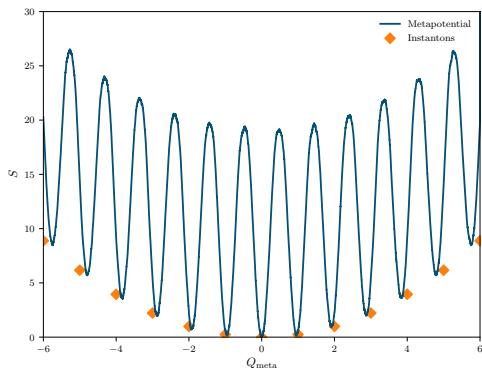
Instanton update - Action difference



Instanton actions - U(1) vs SU(3)

2D U(1)

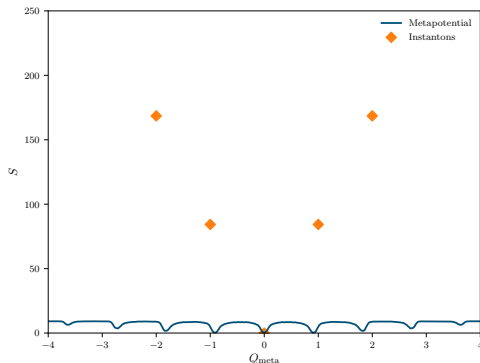
$$V = 32^2, \beta = 12.8$$



$$S_{\min, Q} = \beta V \left(1 - \cos(2\pi V^{-1} |Q|) \right)$$

4D SU(3)

$$V = 22^4, \beta = 6.4035$$



$$S_{\min, Q} = \frac{8\pi^2}{g^2} |Q| = \frac{\beta}{6} 8\pi^2 |Q|$$

Instanton updates + gradient flow

Combination of instanton updates and gradient flow?

- Apply gradient flow
- Multiply flowed configuration with instanton
- Flow back to flowtime 0
- During accept-reject

$$p = \exp(-\Delta S + \ln(\det(\mathcal{J})))$$

⇒ Even lower acceptance probabilities than without flow



OUTLOOK

Outlook & Future plans

For now focus on Metadynamics

- More statistics and parameter tuning!
- Study metadynamics for improved actions
- Guess/fit potential
- Well-tempered Metadynamics (weight changes adaptively \Rightarrow usually better convergence of potential)
- Choosing a better collective variable:
 - Build up variational basis of observables at different scales
 - GEVP to extract leading modes of Markov chain
 - Collective variable from linear combination?
- Multiple timescale integration?

Thank you for your attention!

timo.eichhorn@protonmail.com





BACKUP SLIDES

Well-tempered Metadynamics

[Barducci' 08]

- Original Metadynamics

$$V_{t+1}(Q) = V_t(Q) + w \exp\left(-\frac{(Q_t - Q)^2}{2\sigma^2}\right)$$

- Well-tempered Metadynamics

$$V_{t+1}(Q) = V_t(Q) + \exp\left(-\frac{V_t(Q)}{\Delta T}\right) w \exp\left(-\frac{(Q_t - Q)^2}{2\sigma^2}\right)$$

Tunable parameter ΔT :

- $\Delta T \rightarrow 0$: No Metadynamics
- $\Delta T \rightarrow \infty$: Original metadynamics

Construction of SU(3) instantons

Based on [Jahn' 19]

- Construction of instanton with radius ρ centered around z
- Embed SU(2) BPST instantons into SU(3)
- In singular gauge the vector potential is given by

$$A_\mu = \eta_{a\mu\nu} \frac{\rho^2 (x_\nu - z_\nu) \tau_a}{(x - z)^2 ((x - z)^2 + \rho^2)}$$

- Deal with periodicity/boundary effects by applying 150 stout smearing sweeps with $\rho_{\text{stout}} = 0.12$
- For an anti-instanton replace the 't Hooft symbol $\eta_{a\mu\nu}$ with an anti 't Hooft symbol $\bar{\eta}_{a\mu\nu}$