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

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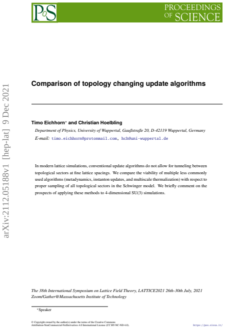
# Introduction

Continuation of [2112.05188]
2D U(1) → 4D SU(3)





Related talks:

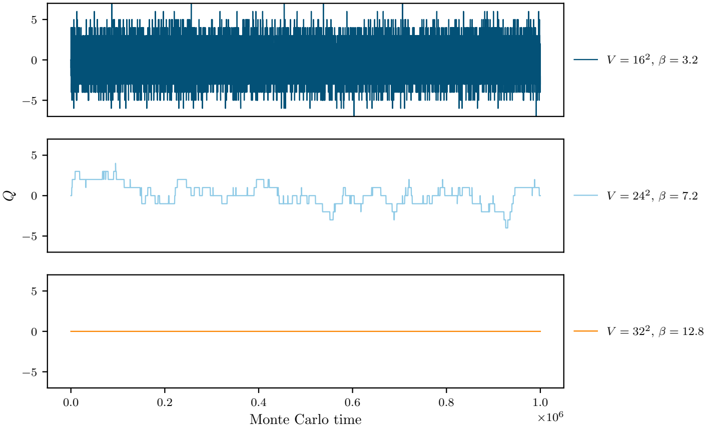
- Parallel tempering: [talk by Ruben Kara]
- Tempered boundaries: [talk by Claudio Bonanno]
- Multicanonical: [talk by Francesco D'Angelo]
- Many more in this session: [Algorithms I] [Algorithms II] [Algorithms III] [Algorithms IV]

Also see [poster by Philip Rouenhoff]

# Motivation

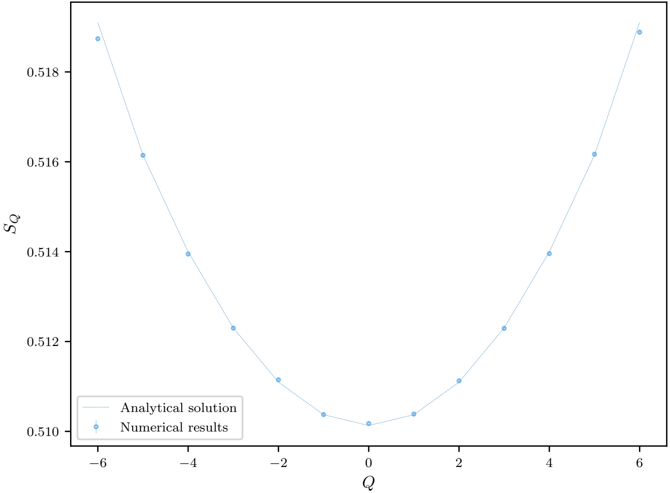
# Topological freezing in 2-dimensional U(1)

Not exclusive to QCD/SU(3) gauge theory

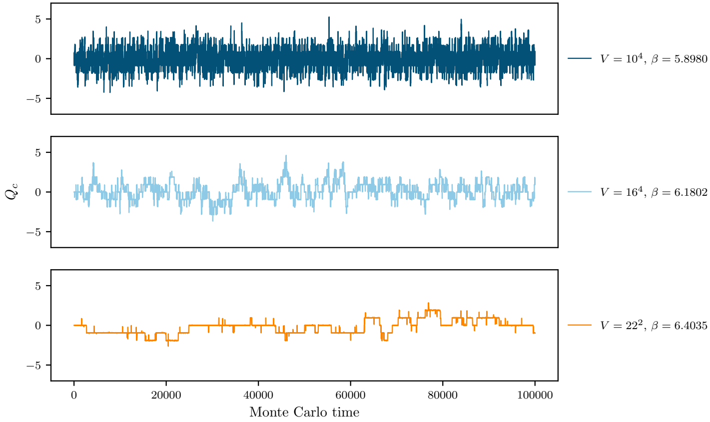


# Topological freezing - Consequences

Slow topological modes couple to other observables!

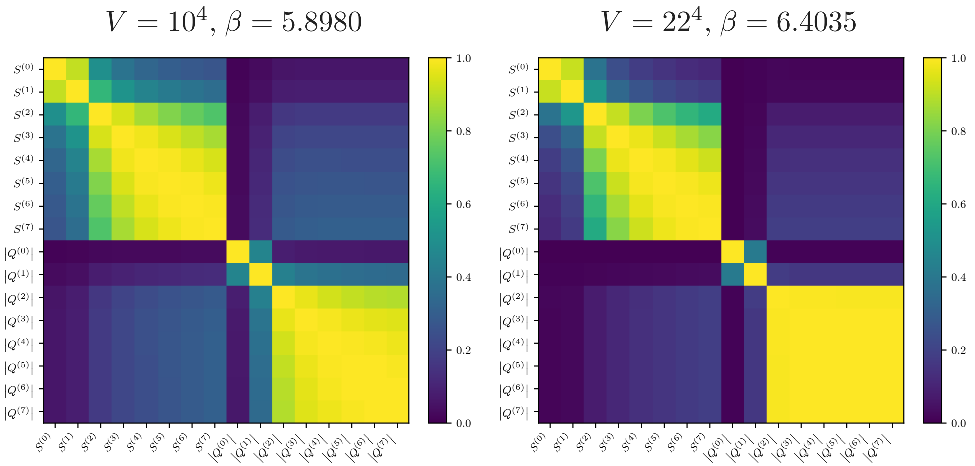


# Topological freezing in 4-dimensional SU(3)



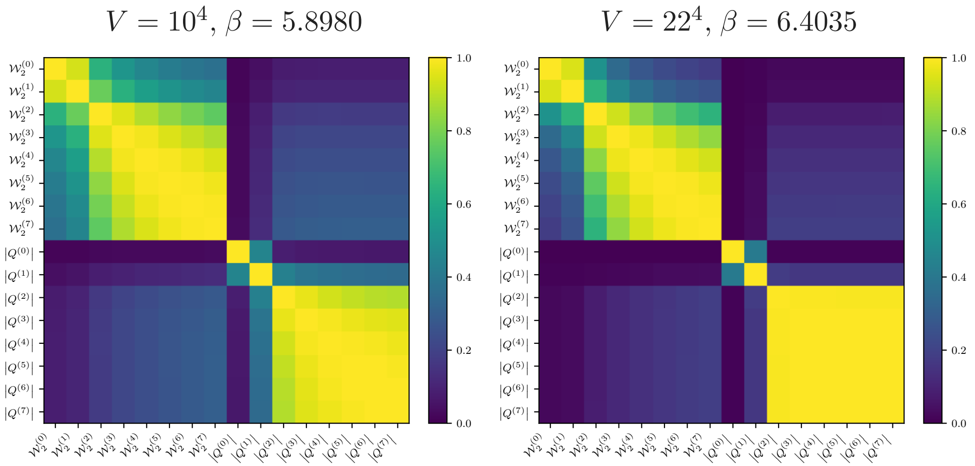

Not yet completely frozen for the lattice spacings considered here

# Topological freezing - Consequences



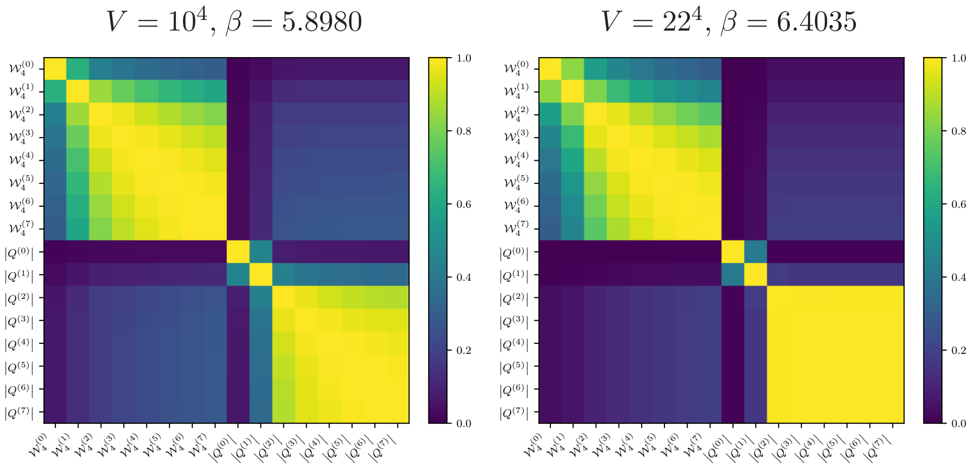

Weak but non-vanishing correlation between action and topological charge!

# Topological freezing - Consequences



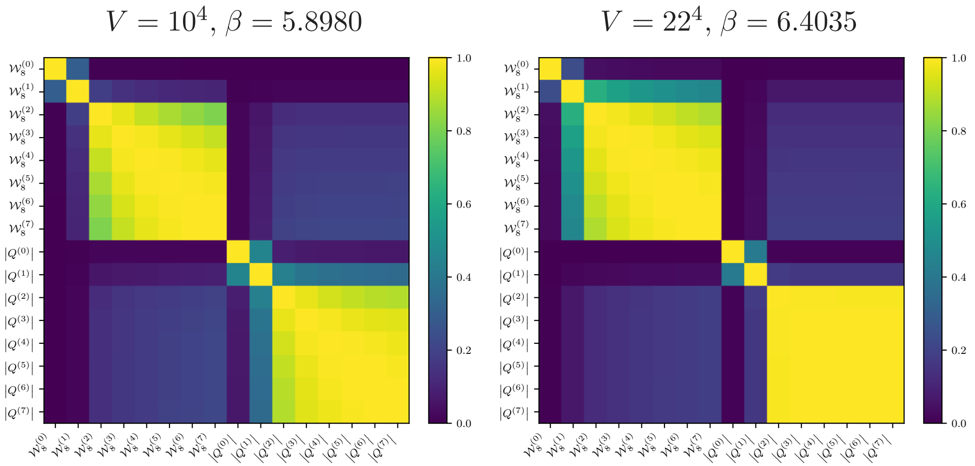

The same can be seen for Wilson loops ($L = 2$)

# Topological freezing - Consequences




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

# Topological freezing - Consequences




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

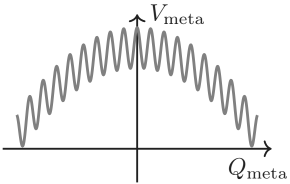
# Update algorithms

# Two approaches

## Metadynamics

[Laio et al '16]

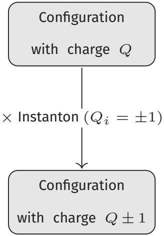
Add history-dependent bias potential to action




## Instanton updates

[Fucito et al '84]

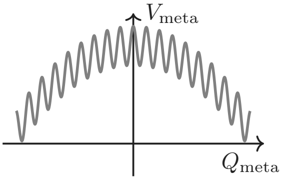
Multiply configurations with instantons



# Metadynamics

**Metadynamics**

[Laio et al '16]
Add history-dependent bias potential to action




- Requires non-integer definition of $Q$:

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

  Here: Clover-definition with under-smeared fields
- After every accepted update, also update $V_{\text{meta}}$
- Add bias potential to action

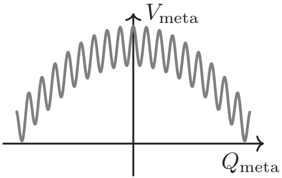
$$S_{\text{meta}} = S_g + V_{\text{meta}}$$

- Reweight observables back to desired distribution

# Metadynamics

**Metadynamics**

[Laio et al '16]
Add history-dependent bias potential to action



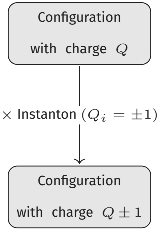

- Local update algorithms not feasible:
  - **Heatbath + Overrelaxation:** No force induced by Metadynamics, doesn't help with tunneling
  - **Metropolis:** Either compute $\Delta Q_{\text{meta}}$ for every link update (too expensive) or after one sweep (low acceptance rate)
- Use global updates (**Hybrid Monte Carlo**): $\Rightarrow$ 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**

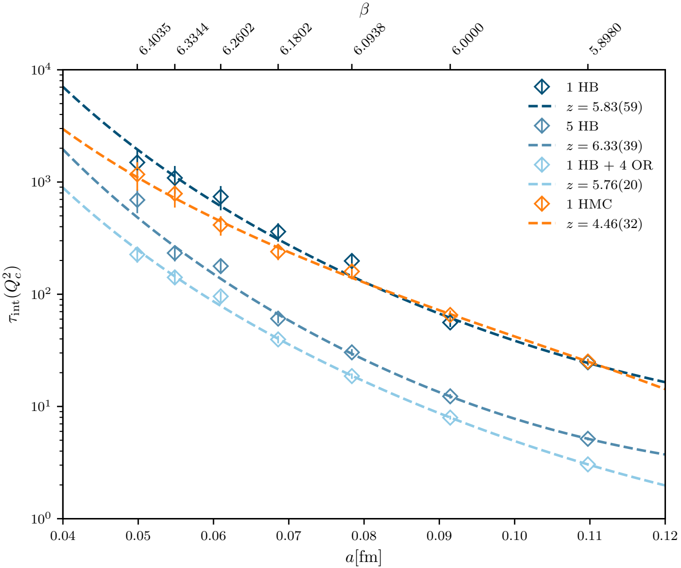
[Fucito et al '84]
Multiply configurations with instantons




- 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
  $\Rightarrow$ Advantage: No need to pass through phase space regions with high action

# Results
## Conventional updates

# Conventional update algorithms



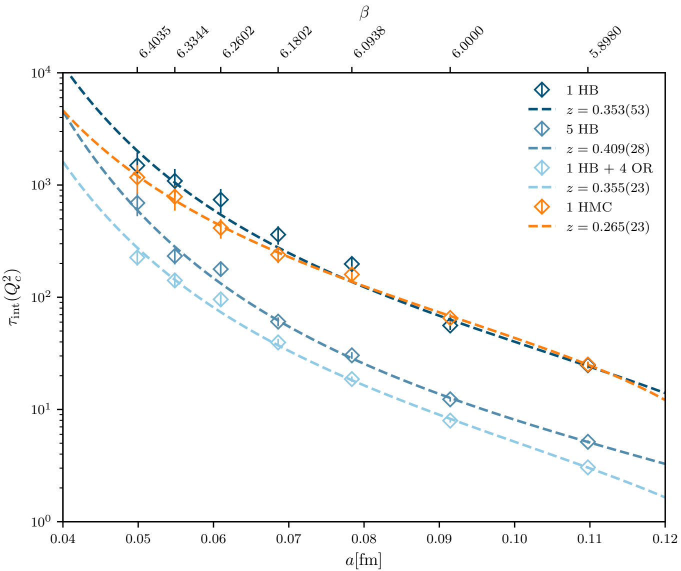

- **HB:** Heatbath over 3 SU(2) subgroups
- **OR:** Overrelaxation over 3 SU(2) subgroups
- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

**Topological charge**

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

$$z \approx 5 - 6?$$

# Conventional update algorithms



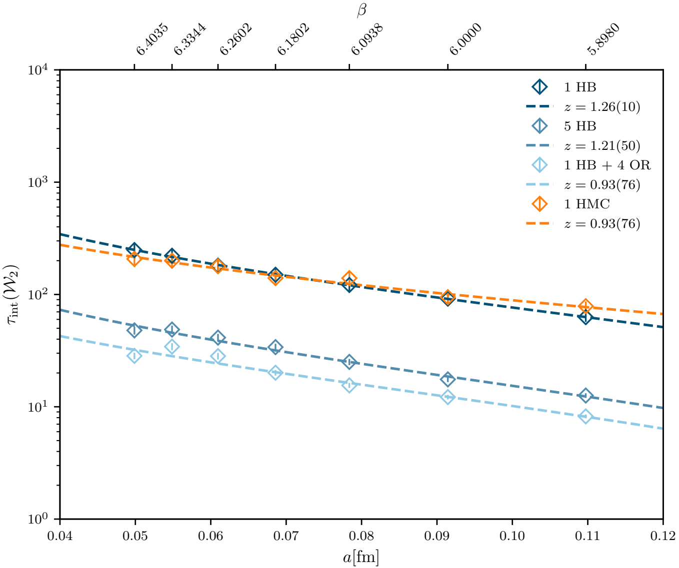

- **HB:** Heatbath over 3 SU(2) subgroups
- **OR:** Overrelaxation over 3 SU(2) subgroups
- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

**Topological charge**

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

$$z \approx 0.2 - 0.4?$$

# Conventional update algorithms



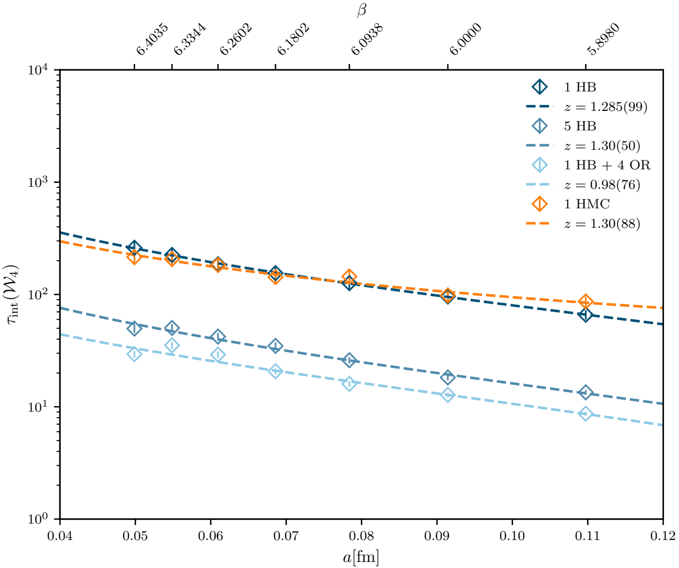

- **HB:** Heatbath over 3 SU(2) subgroups
- **OR:** Overrelaxation over 3 SU(2) subgroups
- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

**Smeared Wilson loops**

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

$$z \approx 1 - 2?$$

# Conventional update algorithms




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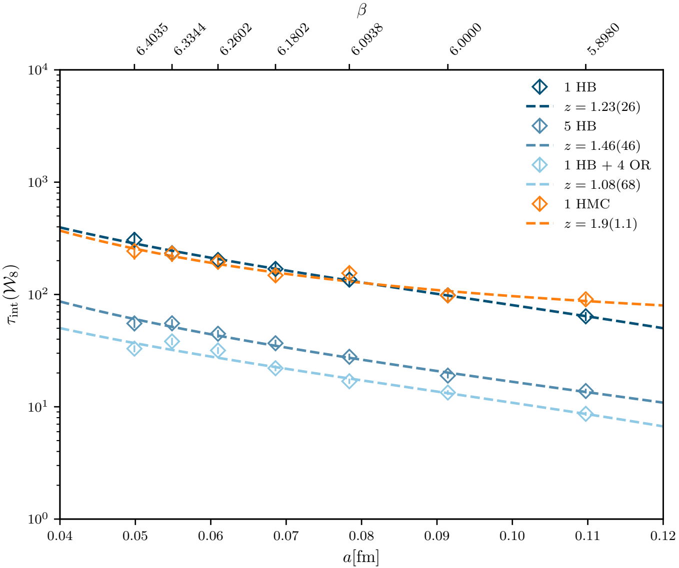
- **HMC:** Unit length Hybrid Monte Carlo with 4th order minimum norm integrator

**Smeared Wilson loops**

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

$$z \approx 1 - 2?$$

# 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

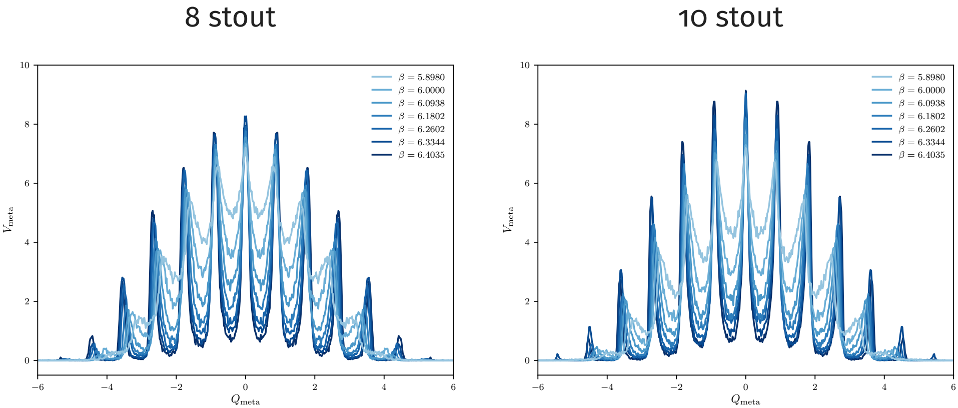
**Smeared Wilson loops**

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

$$z \approx 1 - 2?$$

# Results
# Metadynamics

# Scaling of metapotential

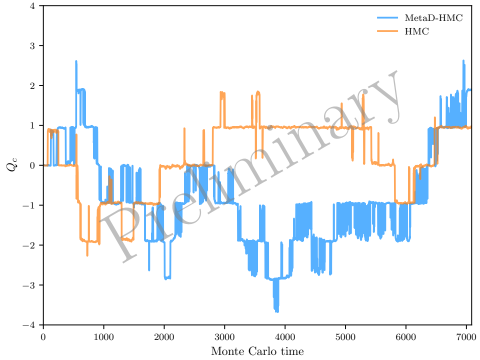



$\Rightarrow$ Smoother potentials (well-tempered Metadynamics or filter?)

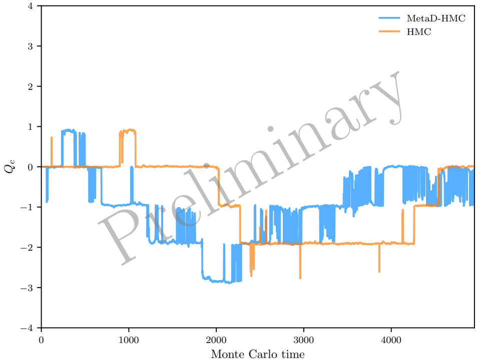
$\Rightarrow$ Tune smearing steps

# Metadynamics timeseries

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

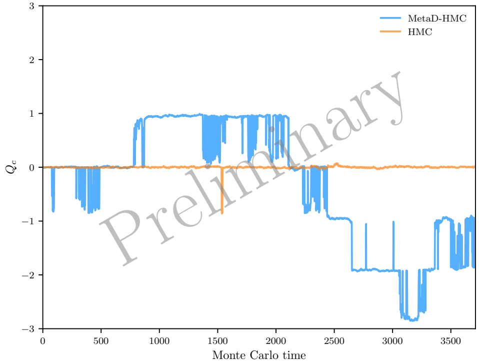



$V = 20^4, \beta = 6.3344$



# Metadynamics timeseries

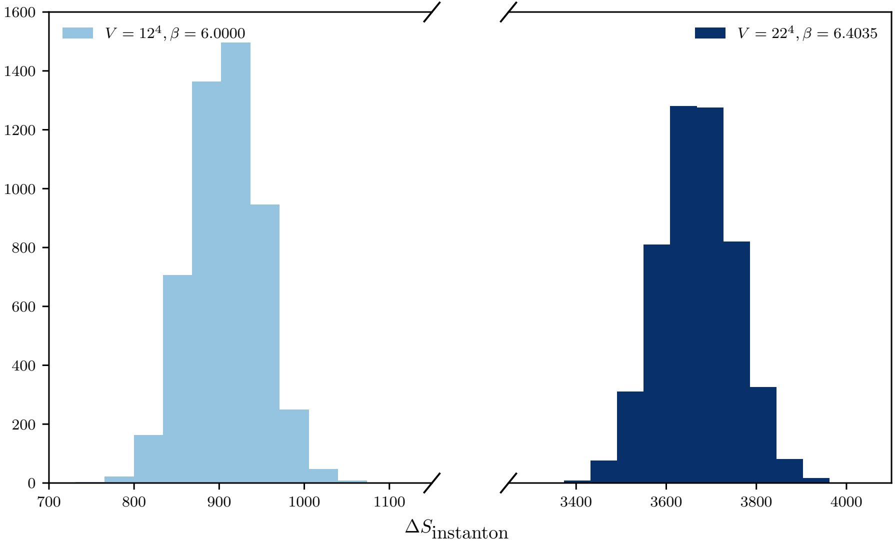
$V = 22^4,\ \beta = 6.4035$




- 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

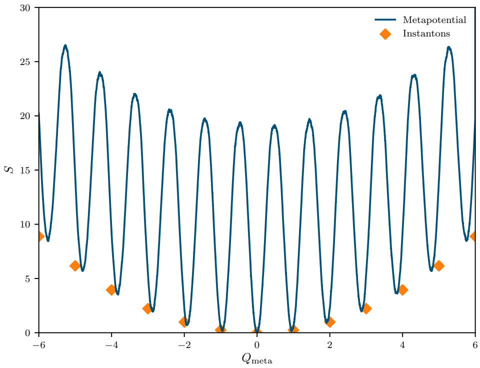
# Instanton update - Action difference



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

2D U(1)

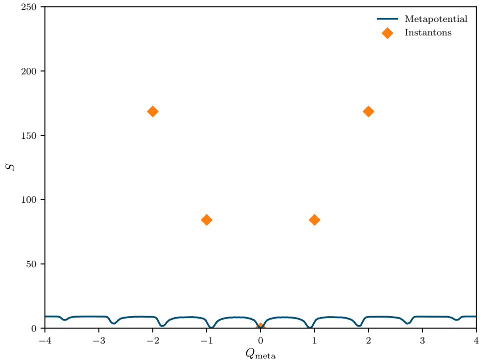
$$V = 32^2, \beta = 12.8$$




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

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

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

$\Rightarrow$ 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!

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# 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 $\Delta T$:

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

# Construction of SU(3) instantons

Based on [Jahn' 19]

- Construction of instanton with radius $\rho$ 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 $\bar{\eta}_{a\mu\nu}$