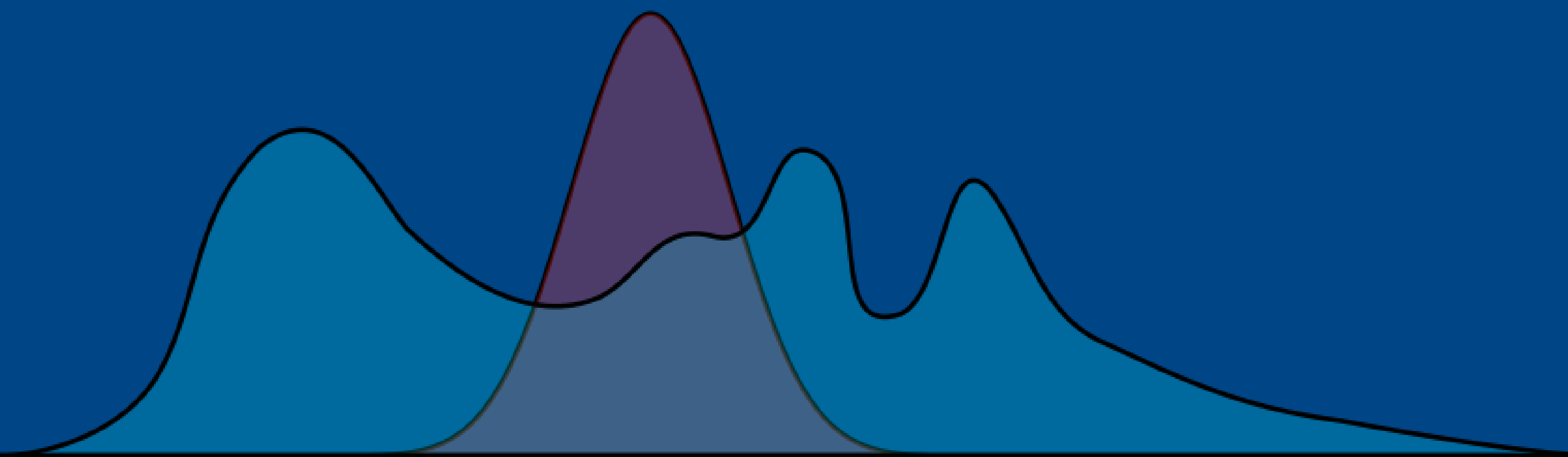

Improved topological sampling for lattice gauge theories

David Albandea

LATTICE21
JULY 26-30 2021, ZOOM/GATHER@MIT

Topological sampling through windings

David Albandea,[1] Pilar Hernández,[1] Alberto Ramos,[1] and Fernando Romero-López[1]

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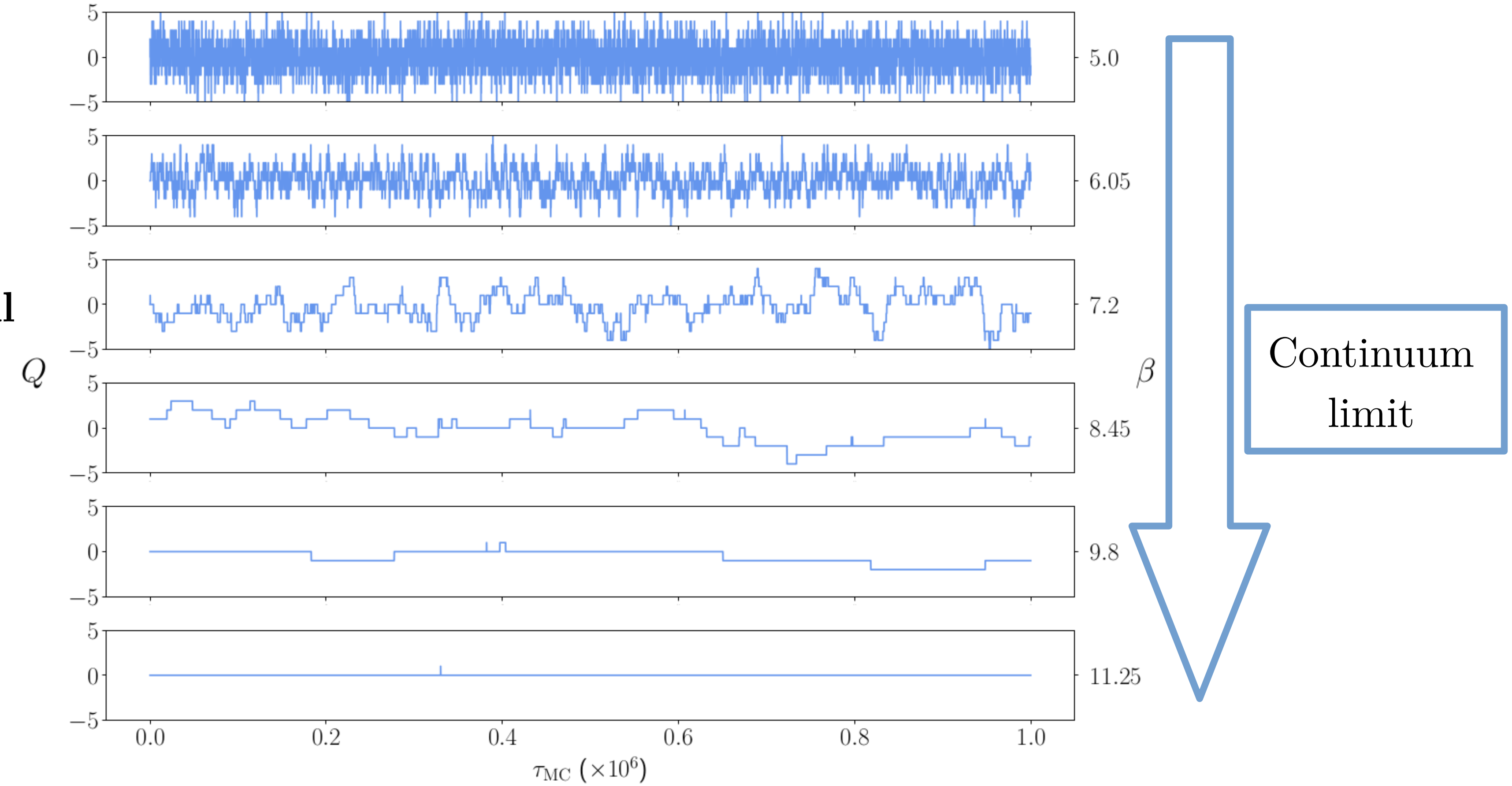
(Dated: June 27, 2021)

We propose a modification of the Hybrid Monte Carlo (HMC) algorithm that overcomes the topological freezing of a two-dimensional $U(1)$ gauge theory with and without fermion content. This algorithm includes reversible jumps between topological sectors—winding steps—combined with standard HMC steps. The full algorithm is referred to as winding HMC (wHMC), and it shows an improved behaviour of the autocorrelation time towards the continuum limit. We find excellent agreement between the wHMC estimates of the plaquette and topological susceptibility and the analytical predictions in the $U(1)$ pure gauge theory, which are known even at finite β. We also study the expectation values in fixed topological sectors using both HMC and wHMC, with and without fermions. Even when topology is frozen in HMC—leading to significant deviations in topological as well as non-topological quantities—the two algorithms agree on the fixed-topology averages. Finally, we briefly compare the wHMC algorithm results to those obtained with master-field simulations of size $L \sim 8 \times 10^3$.

Topology freezing

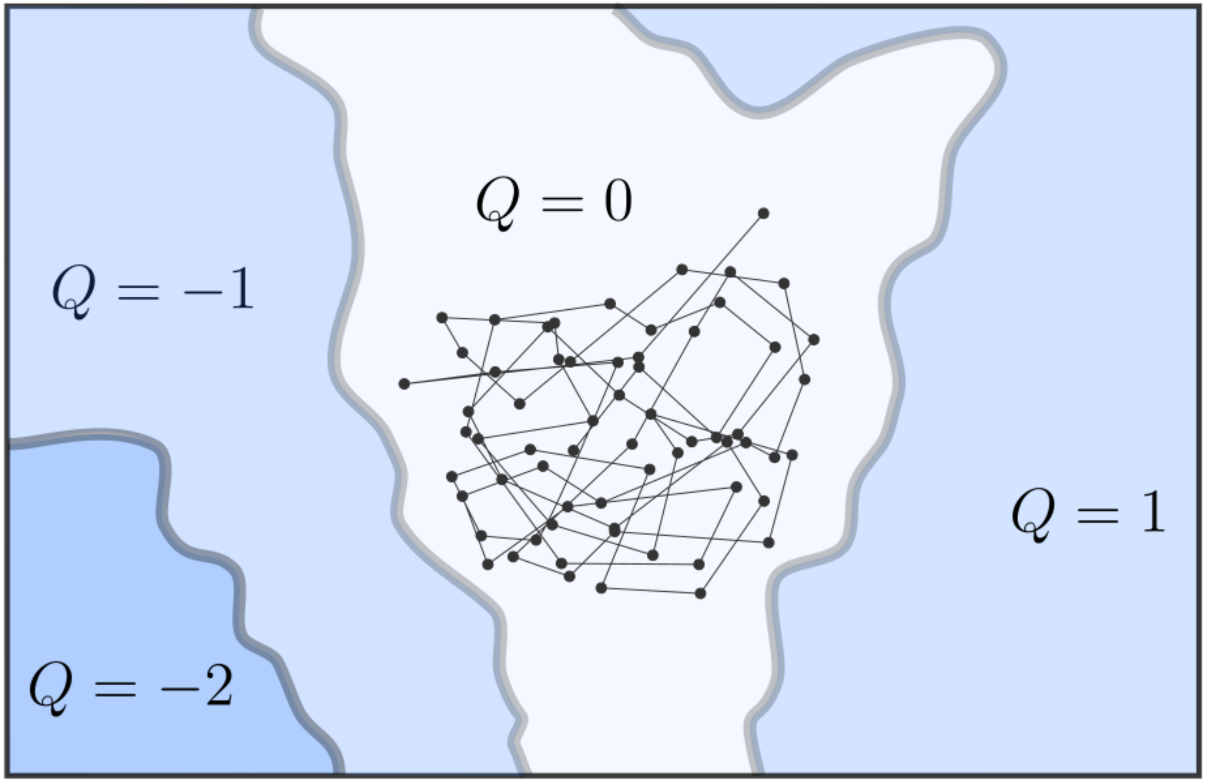
Topological charge histories



☆ Topological charge freezes going to the continuum

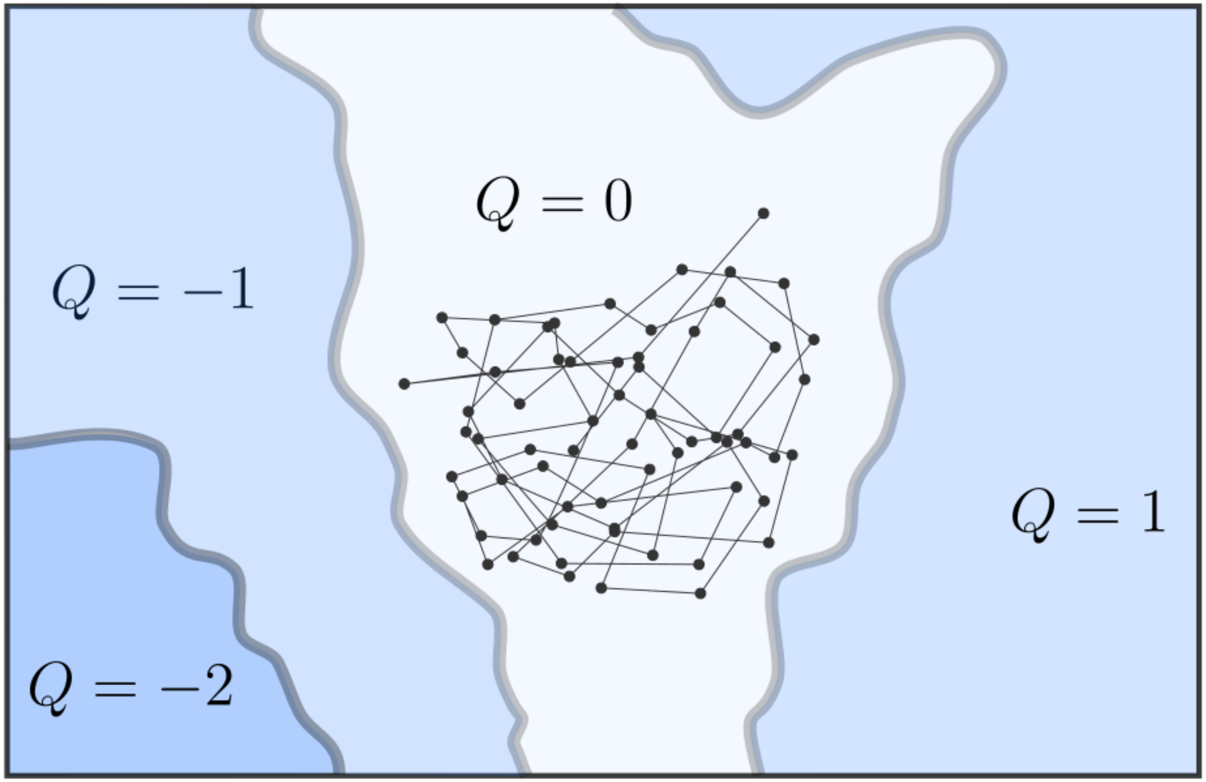
⇨ **Long autocorrelation times**

Topology freezing



☆ HMC proposes configurations with the same Q

Critical Slowing Down



☆ HMC proposes configurations with the same Q

Can we build an algorithm that proposes $Q \to Q \pm 1$?

The model

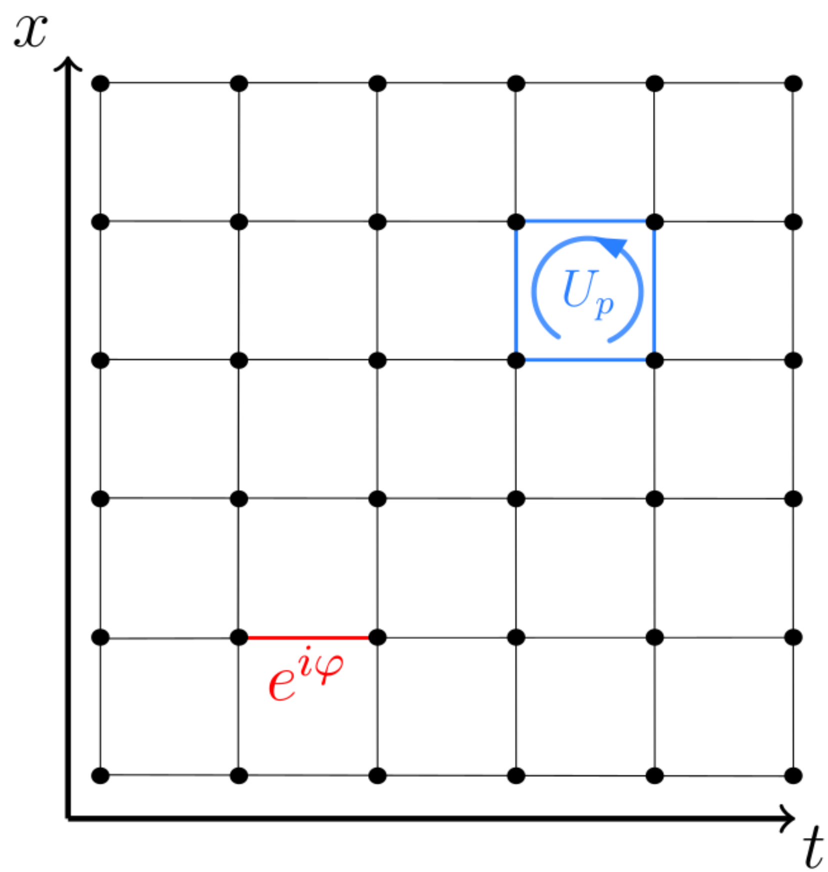
- We worked in U(1) gauge theory in 2D for $N_f = 0$ and $N_f = 2$
  - used as benchmark model in Machine Learning, Tensor Networks...

$$Z = \int \prod_l dU_l \; e^{-S_p[U]} \equiv \int \prod_l dU_l \; e^{\frac{\beta}{2} \sum_p U_p + U_p^\dagger},$$

Nice features:

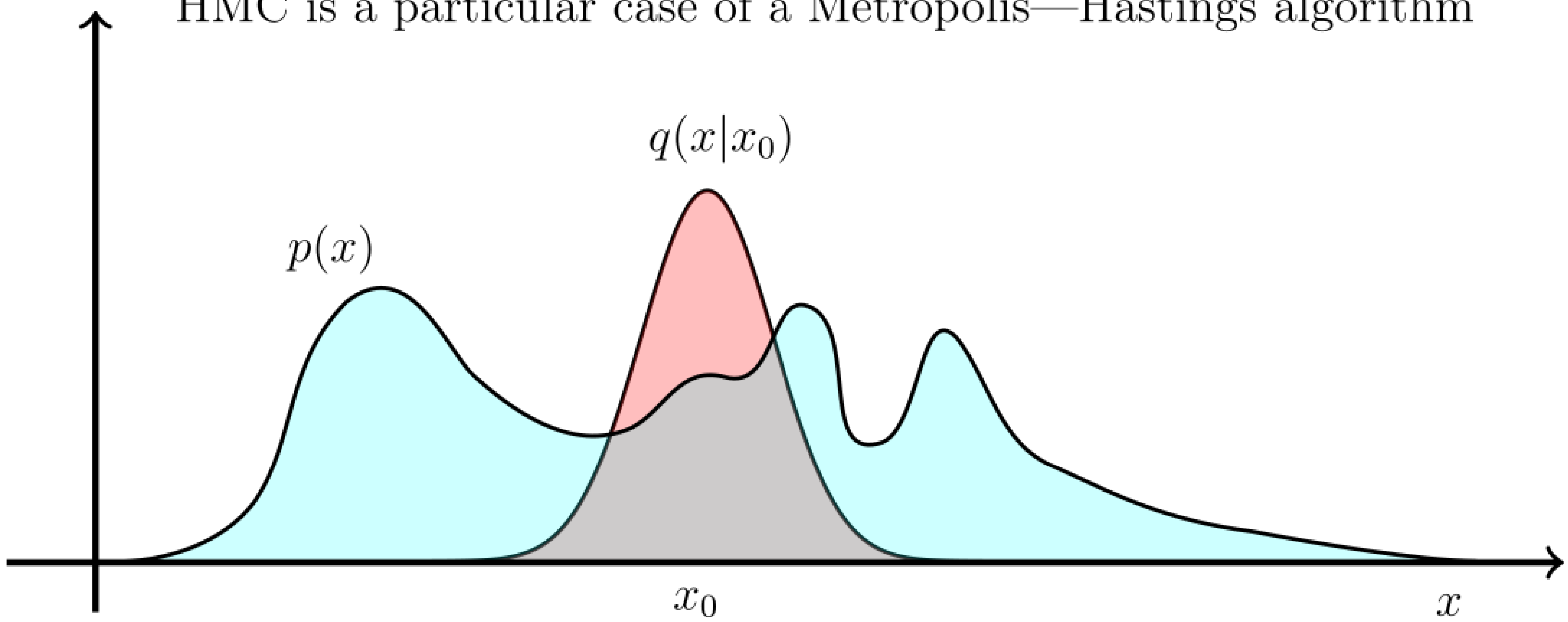
- It is similar to QCD
  - Topology
  - Mass gap ($N_f = 2$)
- Analytical results for $N_f = 0$ at finite β and V
- Topological charge is exactly an integer

$$Q \equiv \frac{-i}{2\pi} \sum_p \ln U_p$$



Hybrid Monte Carlo

HMC is a particular case of a Metropolis—Hastings algorithm



Target distribution

$$p(x) \to e^{-S}$$

Proposal distribution

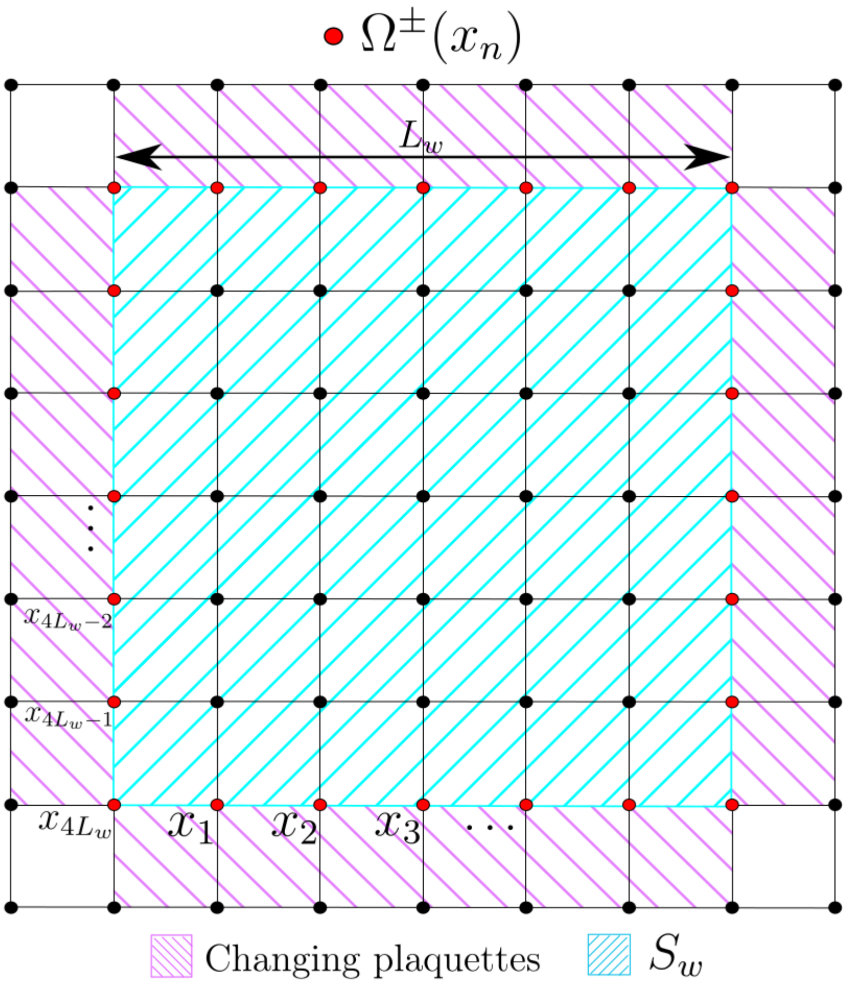
$$q(x'|x) \to \text{Hamilton eqs.}$$

Accept-reject step

$$p_{\text{acc}}(U'|U) = \min\left\{1, \frac{p(U')}{p(U)}\right\}$$

$$\text{with} \quad p(U) = e^{-S[U]}$$

Winding transformation



$$U_\mu(x) \to U_\mu^\Omega(x) \equiv \Omega(x) U_\mu(x) \Omega^\dagger(x+\hat{\mu})$$

if both $x, x+\hat{\mu} \in S_w$

$$\Omega^{\pm}(x_n) = e^{\pm i \frac{\pi}{2} \frac{n}{L_w}}$$

The field $\Omega(x)$ is defined on the boundary of the blue region

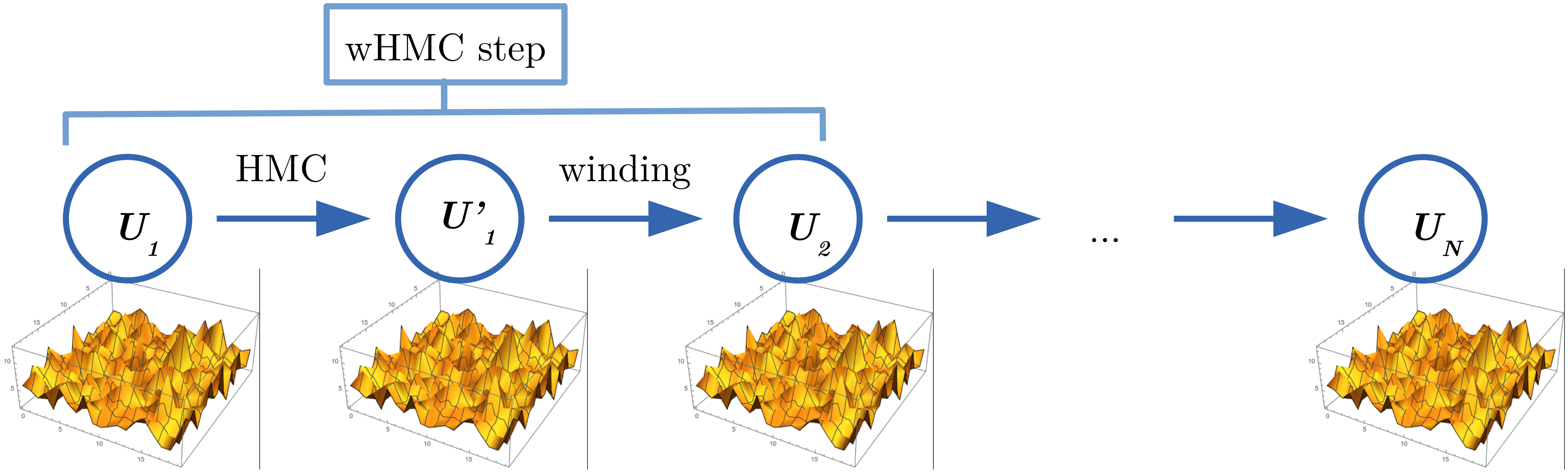
After this, the topological charge is expected to change in one unit
$Q \to Q \pm 1$

Similar to an old attempt under the name of *instanton hit*
F. Fucito and S. Solomon, Phys. Lett. B 134, 230 (1984)
(see also previous talk by Eichhorn)

winding HMC

- ☆ Define the **winding-step** proposal distribution: $q(U'|U) = \frac{1}{2}\delta(U' - U^{\Omega^+}) + \frac{1}{2}\delta(U' - U^{\Omega^-})$

- ☆ Combine HMC and winding transformations ⟹ **wHMC**
  - Satisfies DB
  - Ergodic



winding HMC

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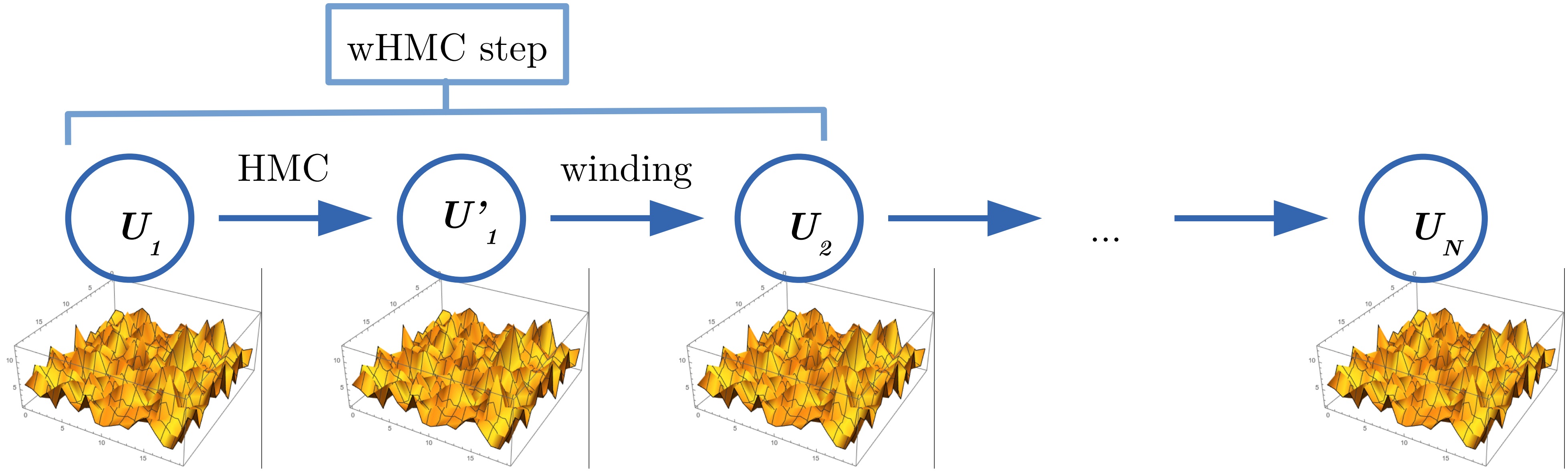
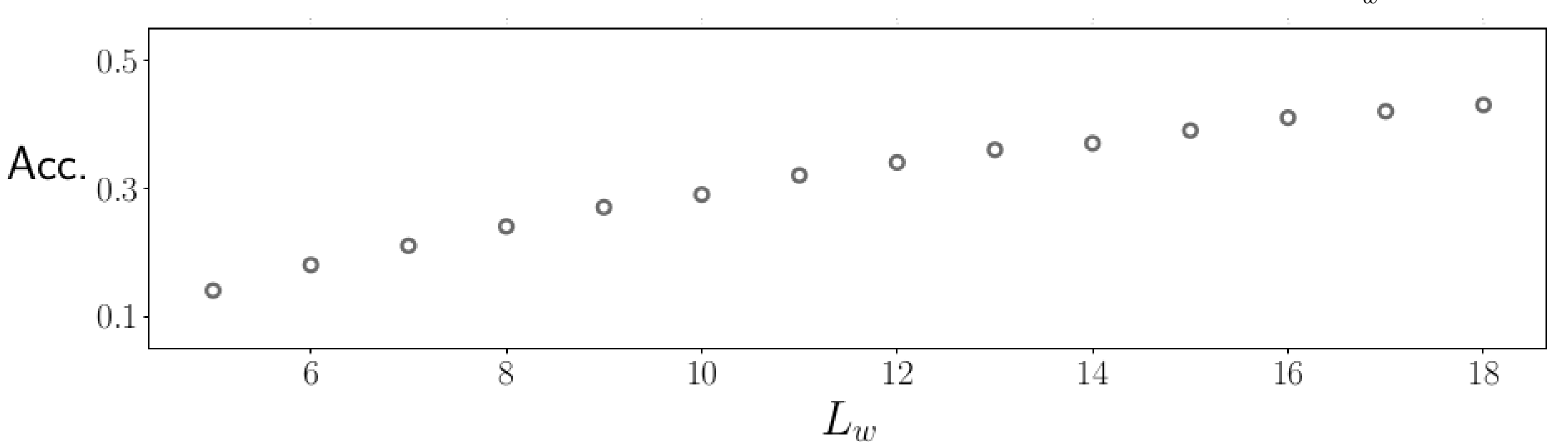


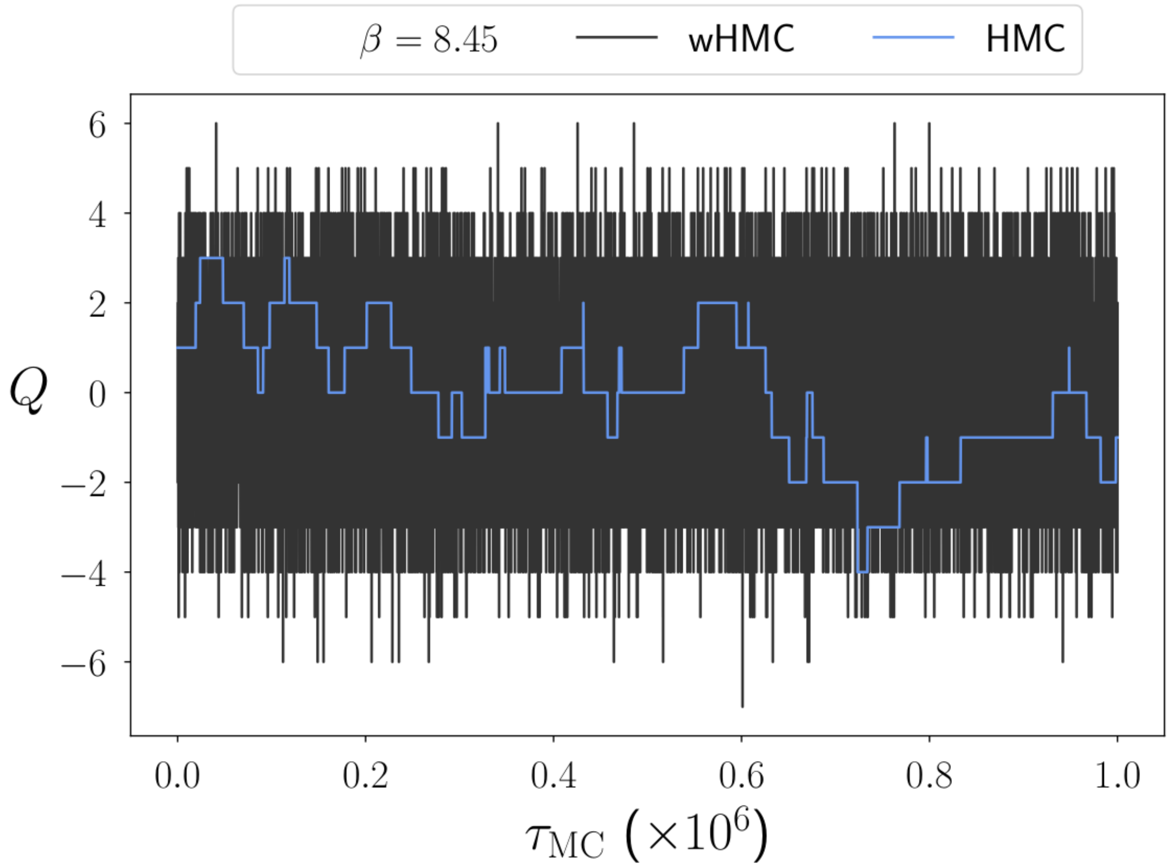
- How does the acceptance of the algorithm change with the size of the winding L_w?

For $N_f = 0$:

$$\langle \Delta S \rangle \simeq \frac{\beta \pi^2}{2 L_w}$$



$N_f = 0$ results

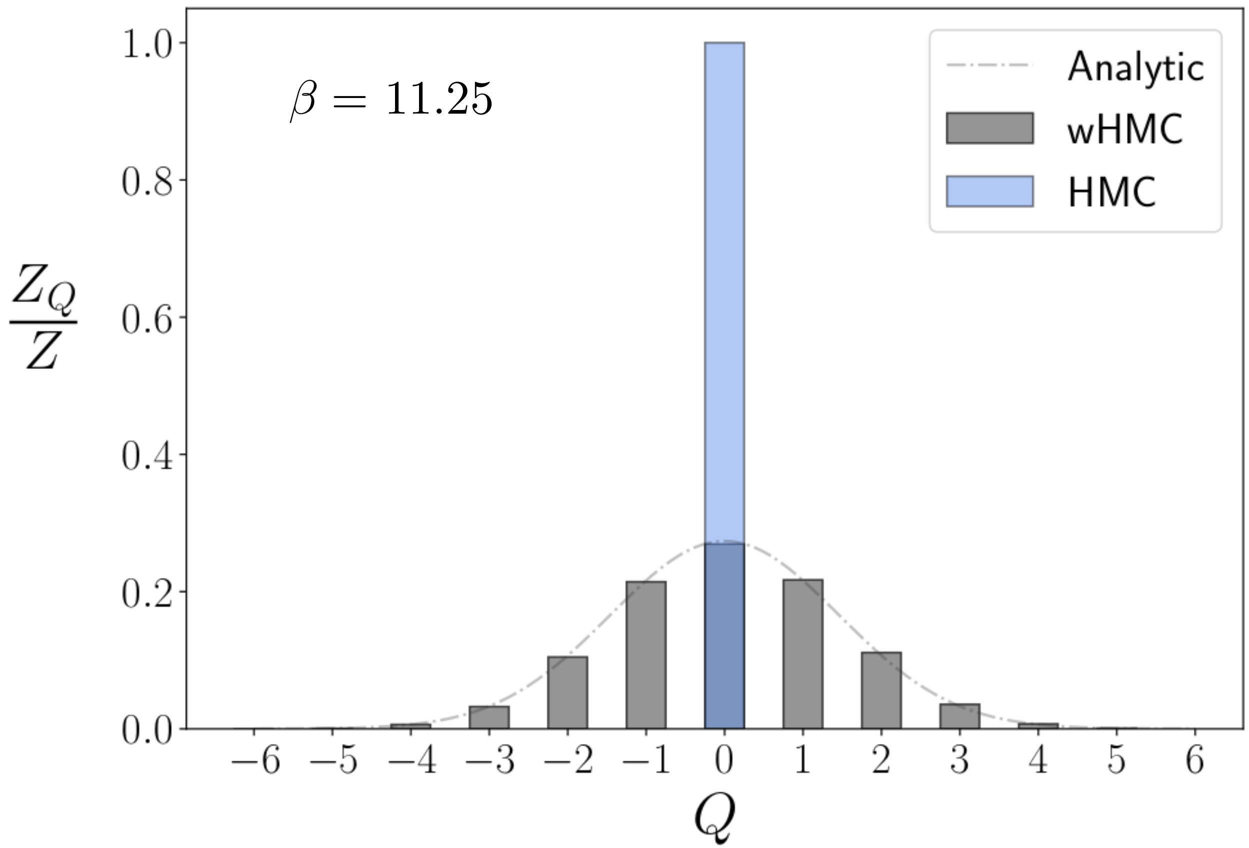


☆ In the pure gauge theory, wHMC samples correctly at β values for which HMC is frozen

⇨ wHMC should lead to correct results

⇨ HMC should lead to incorrect results

$N_f = 0$ results



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$N_f = 0$ results

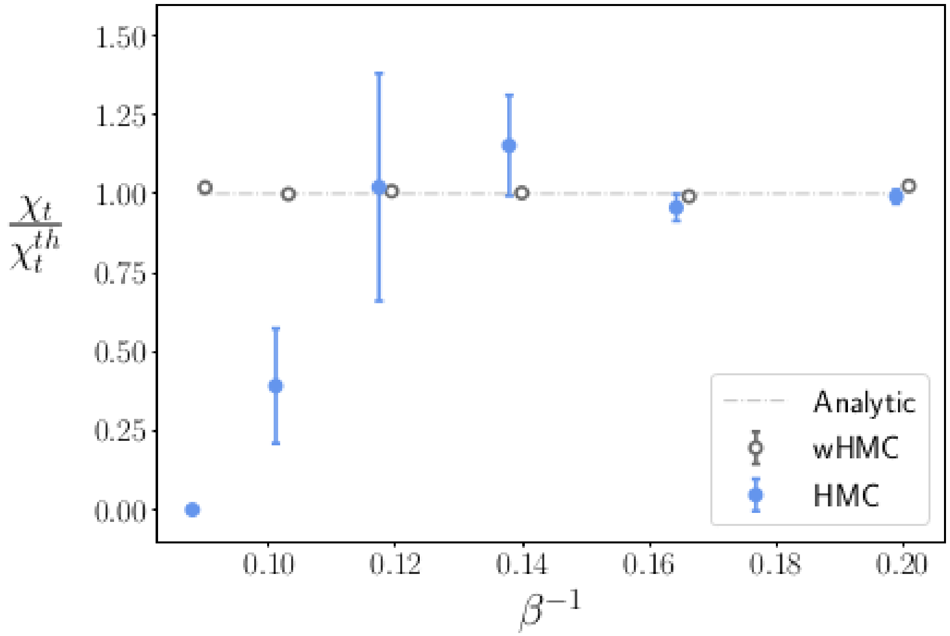
We can check the results of both algorithms for all β

G. Kovács et al., Nucl.Phys. B454 (1995) 45-58 hep-th/9505005
C. Bonati and P. Rossi, Phys. Rev. D **99**, 054503 (2019) 1901.09830
C. Bonati and P. Rossi, Phys. Rev. D **100**, 054502 (2019) 1908.07476

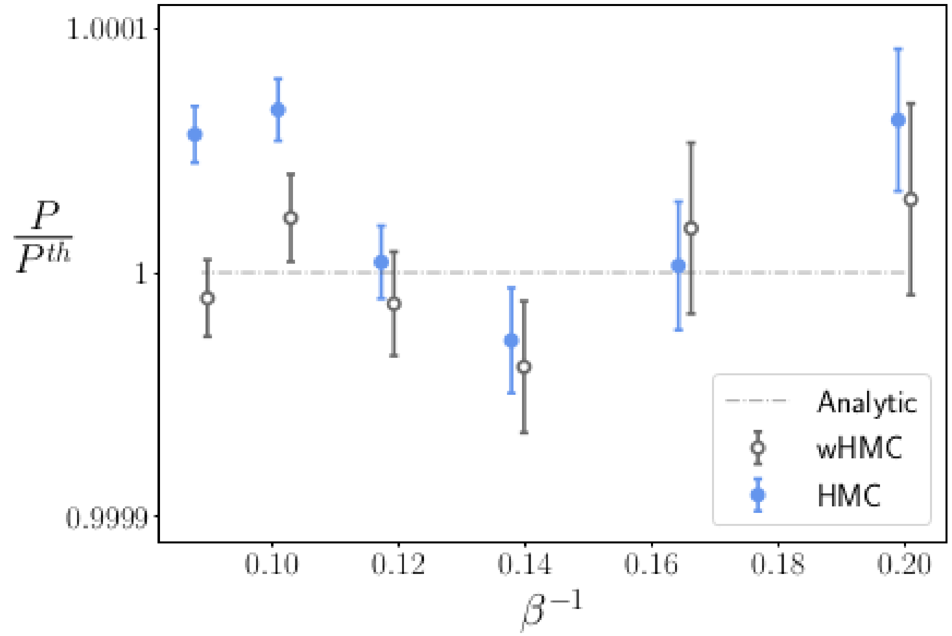
$$\chi_t^{th} = -\frac{\sum_n A_n(\beta) I_n(\beta)^{V-1}}{\sum_n I_n(\beta)^V} - (V-1)\frac{\sum_n B_n^2(\beta) I_n(\beta)^{V-2}}{\sum_n I_n(\beta)^V}$$

$$P^{th} = \frac{\sum_n I_n'[\beta] I_n[\beta]^{V-1}}{\sum_n I_n[\beta]^V}$$

Topological susceptibility



Plaquette



wHMC agrees with analytical results at all β

HMC gets biased approaching the continuum

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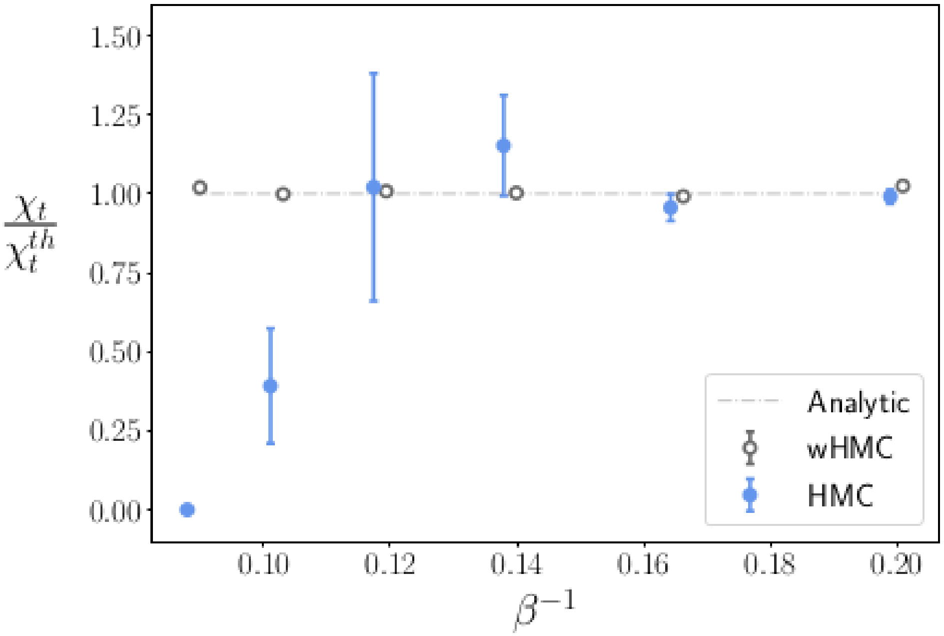
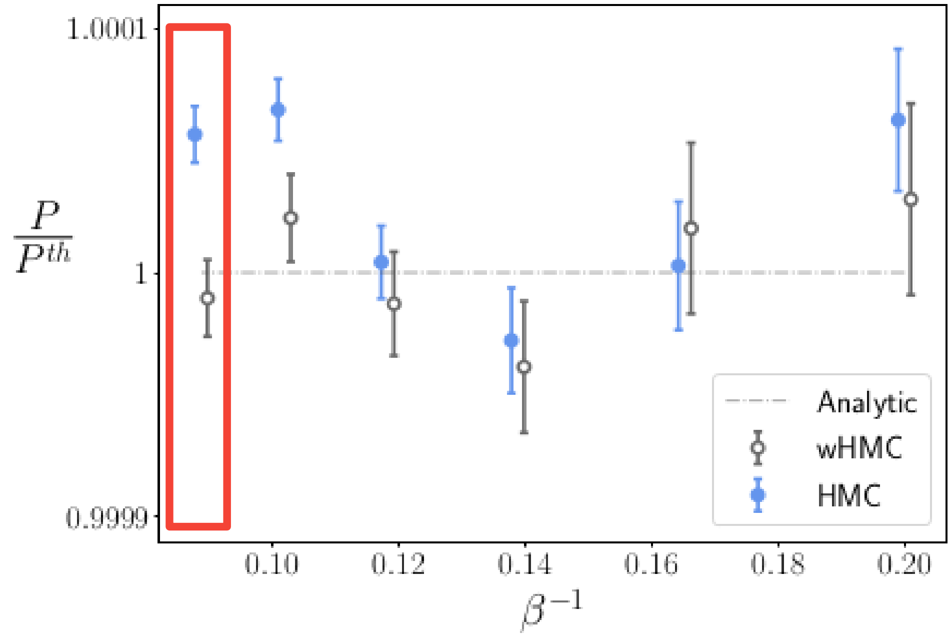




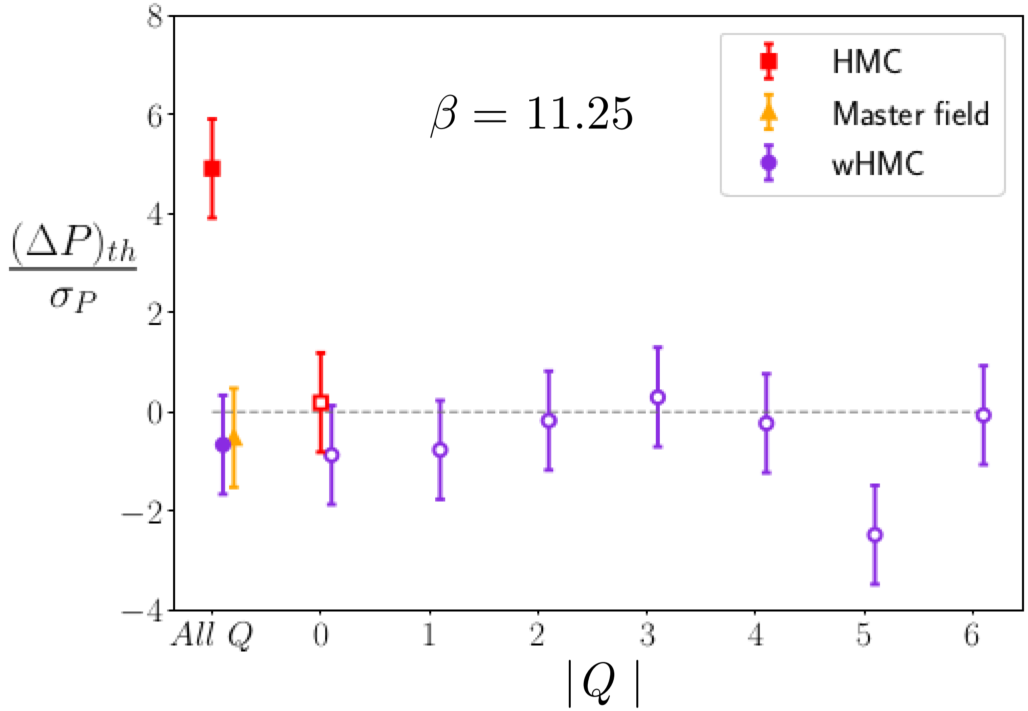
wHMC agrees with analytical results at all β

HMC gets biased approaching the continuum

even for non-topological observables!

$N_f = 0$ results: fixed topology

But does HMC sample correctly observables at fixed topological sectors?



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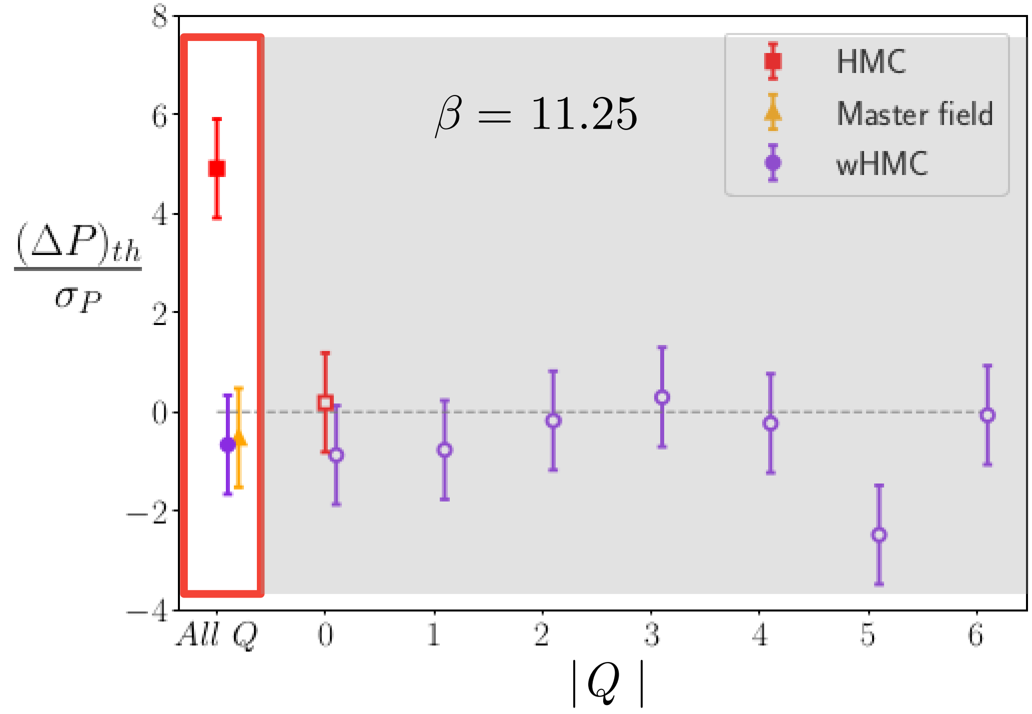

HMC gets wrong the final value of the plaquette

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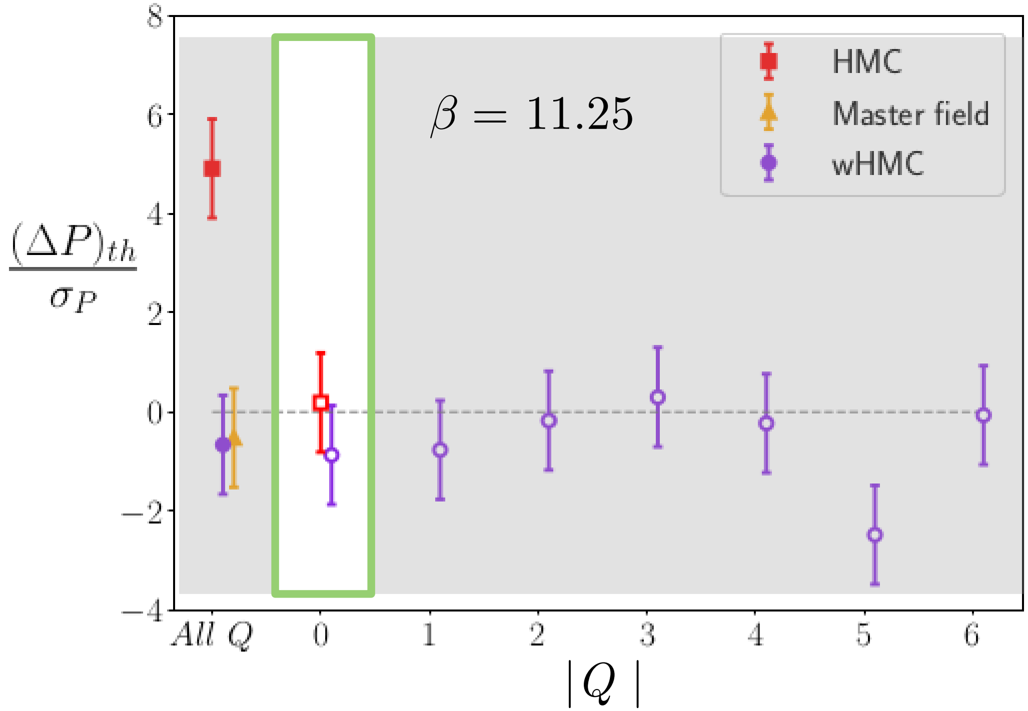
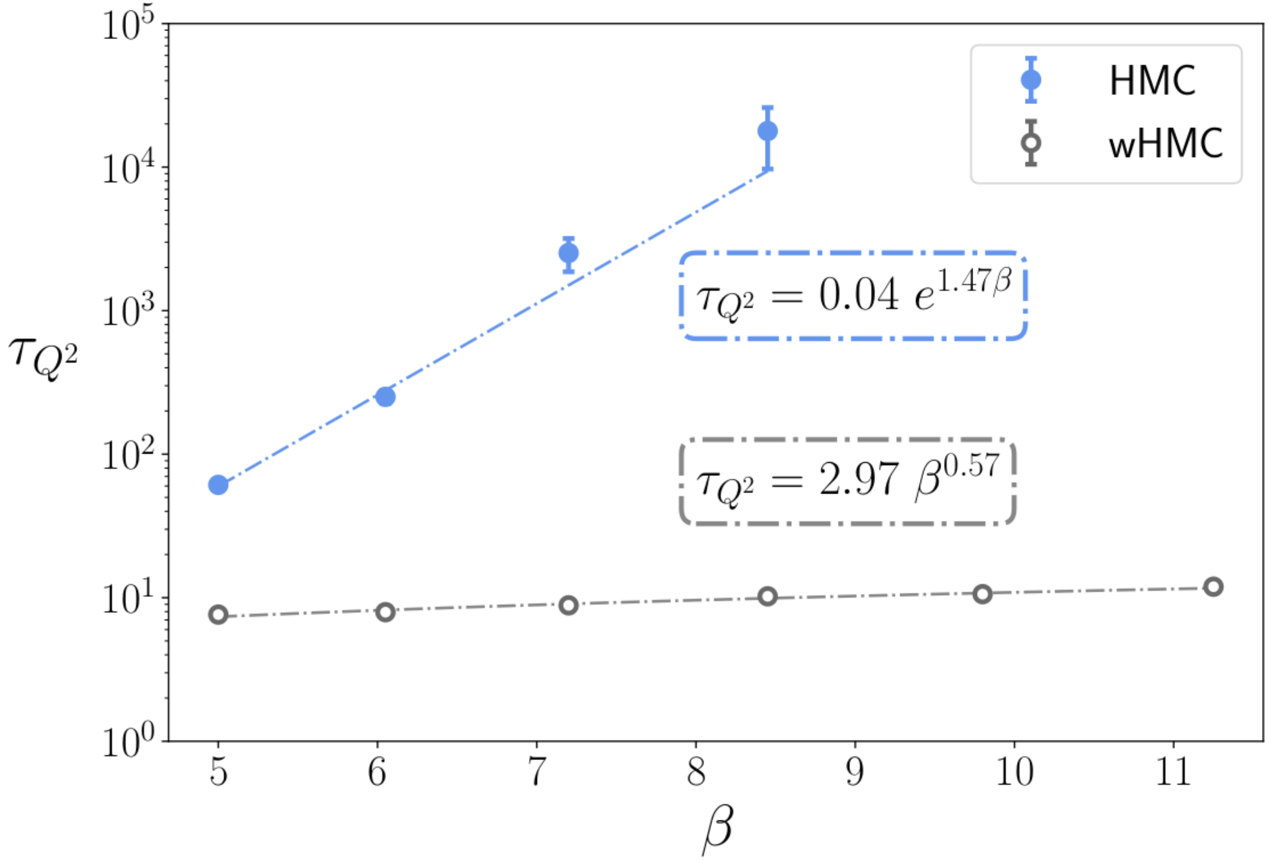


HMC gets wrong the final value of the plaquette

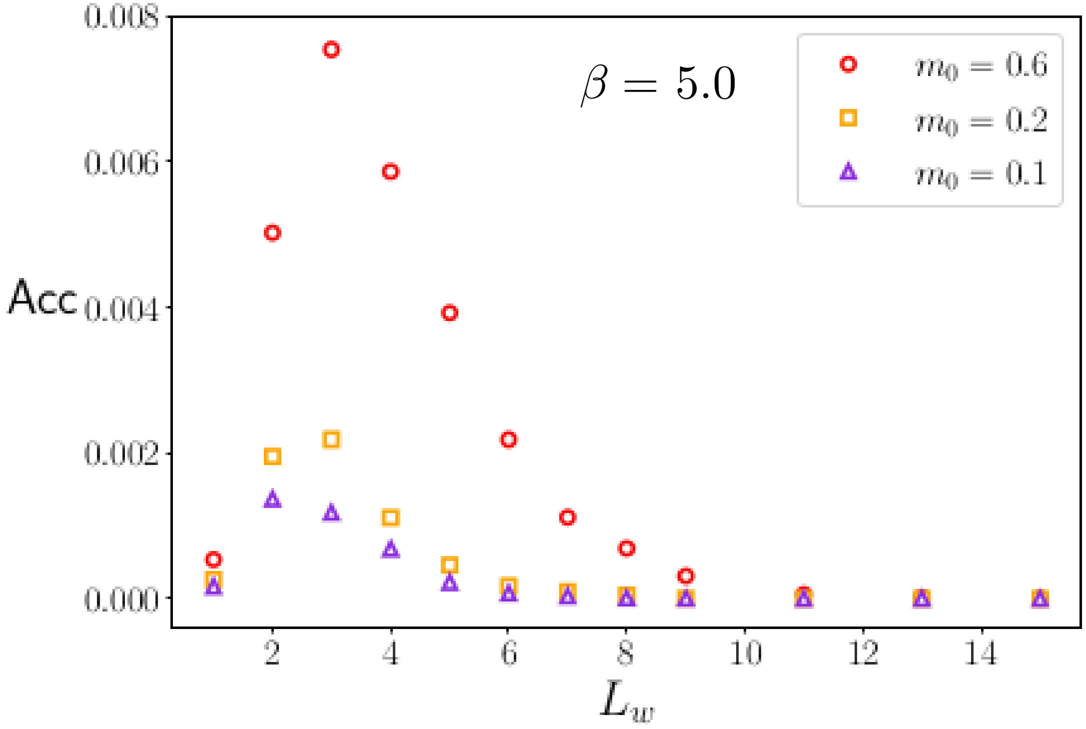
but samples correctly the sector $Q = 0$

$N_f = 0$ results: scaling with a



- HMC autocorrelation increases exponentially
- wHMC increases only polynomially

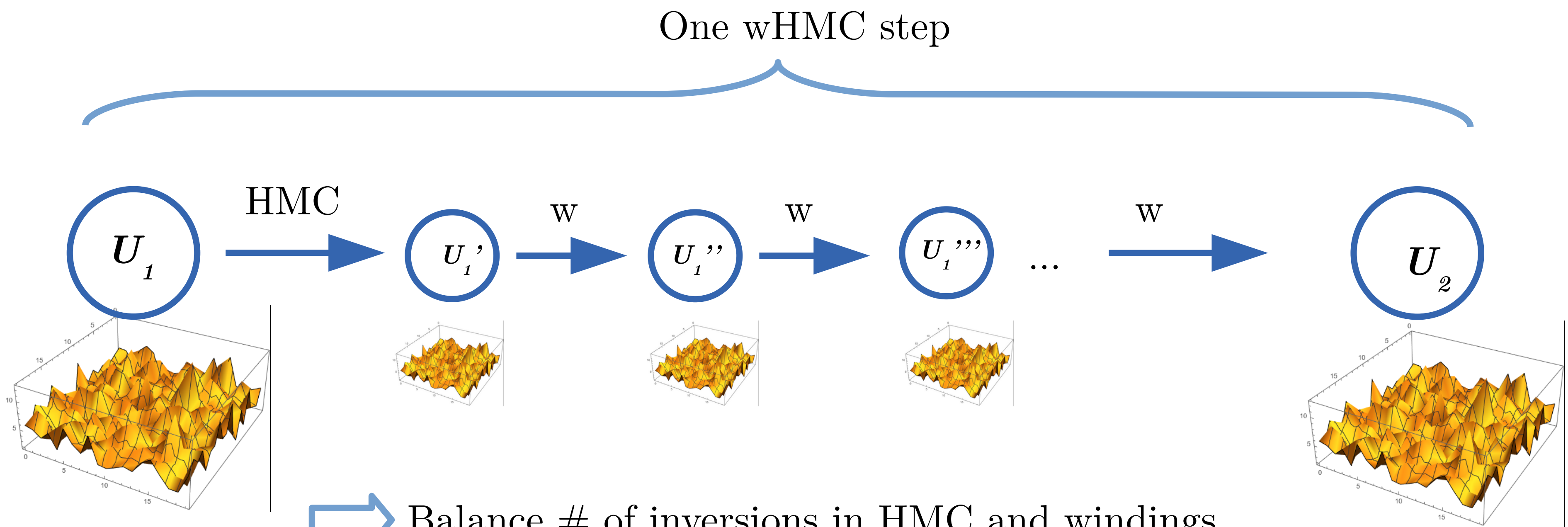
$N_f = 2$



- There is an optimal size for the winding
- Acceptance is much lower

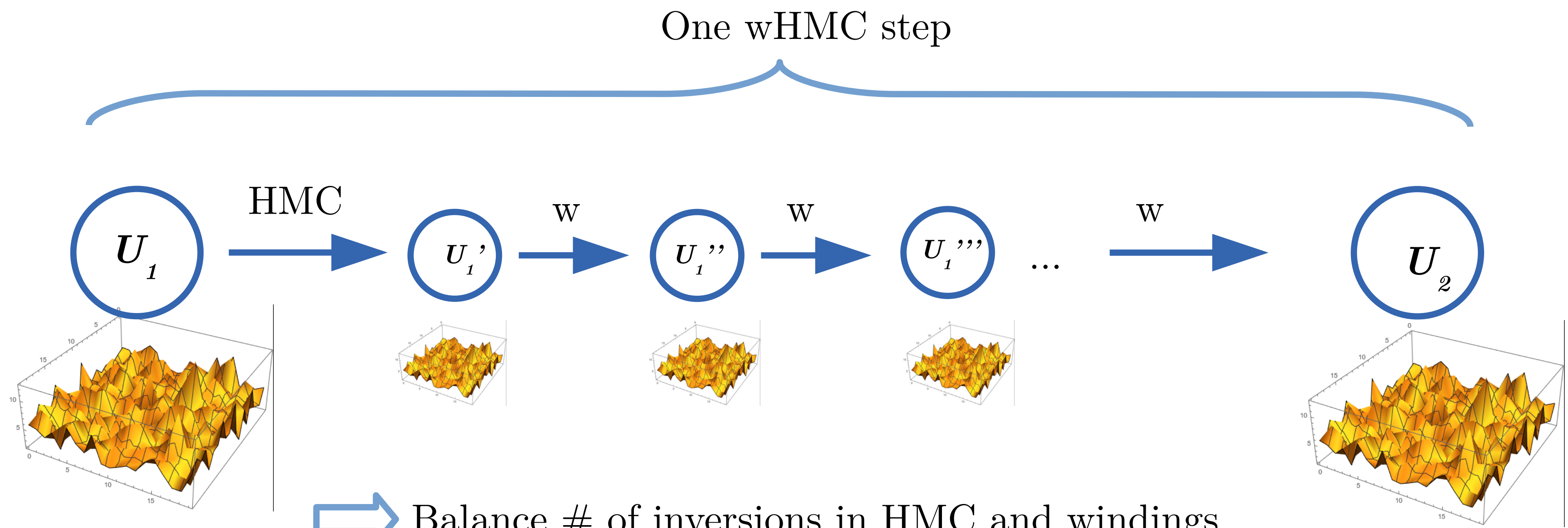
  ⇒ perform several windings per step

$N_f = 2$



⇨ Balance # of inversions in HMC and windings

$N_f = 2$



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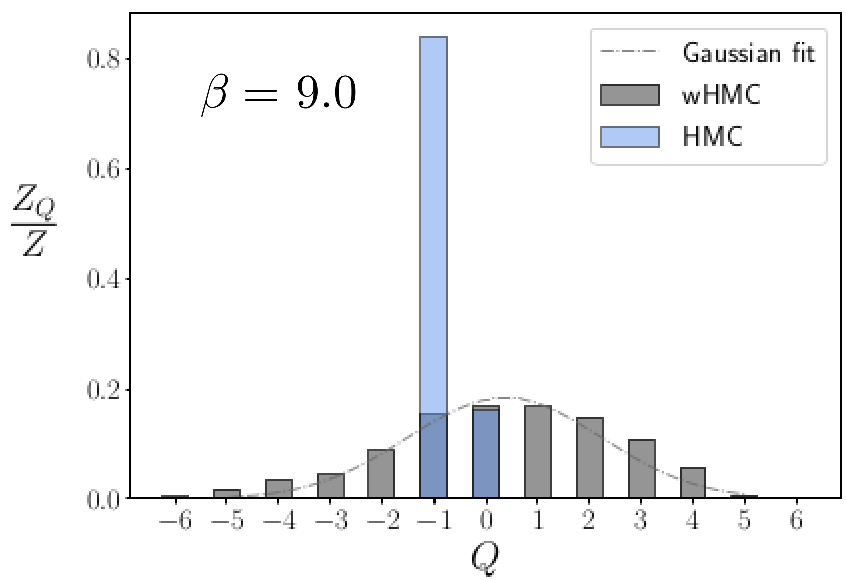
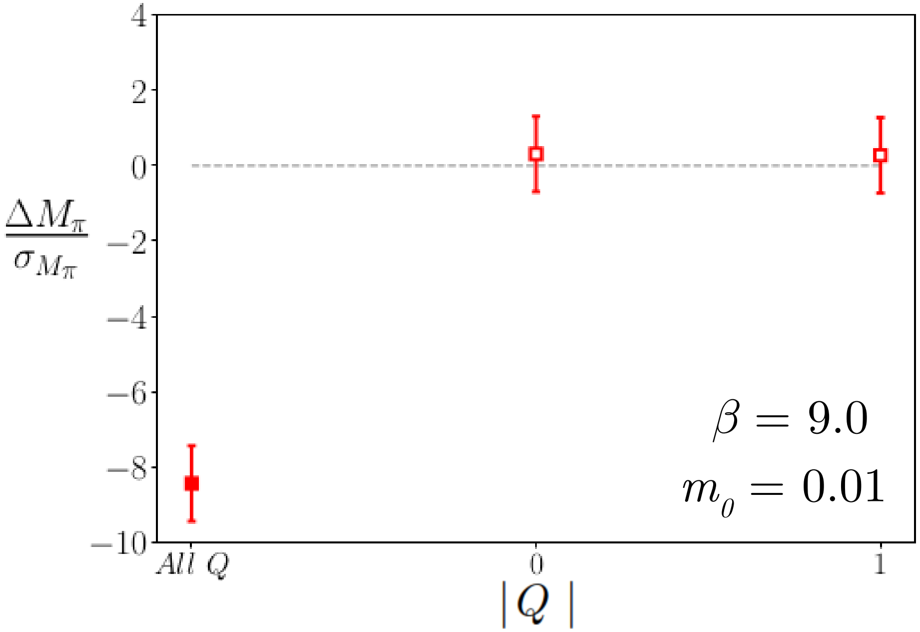


☆ At equivalent computational costs, wHMC is still able to sample all relevant topological sectors

$N_f = 2$ results

Pion Mass discrepancy between wHMC and HMC



$N_f = 2$ results

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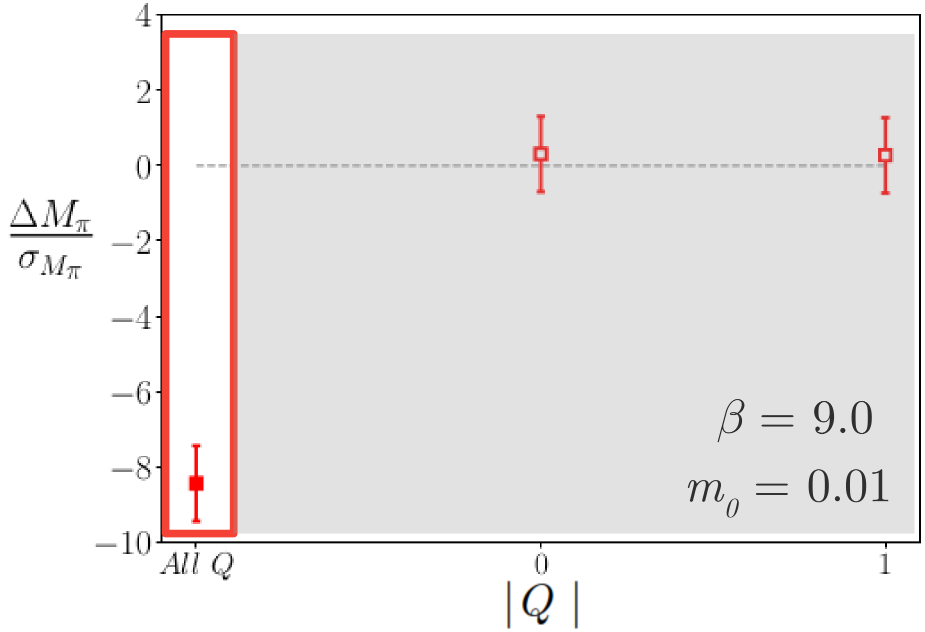
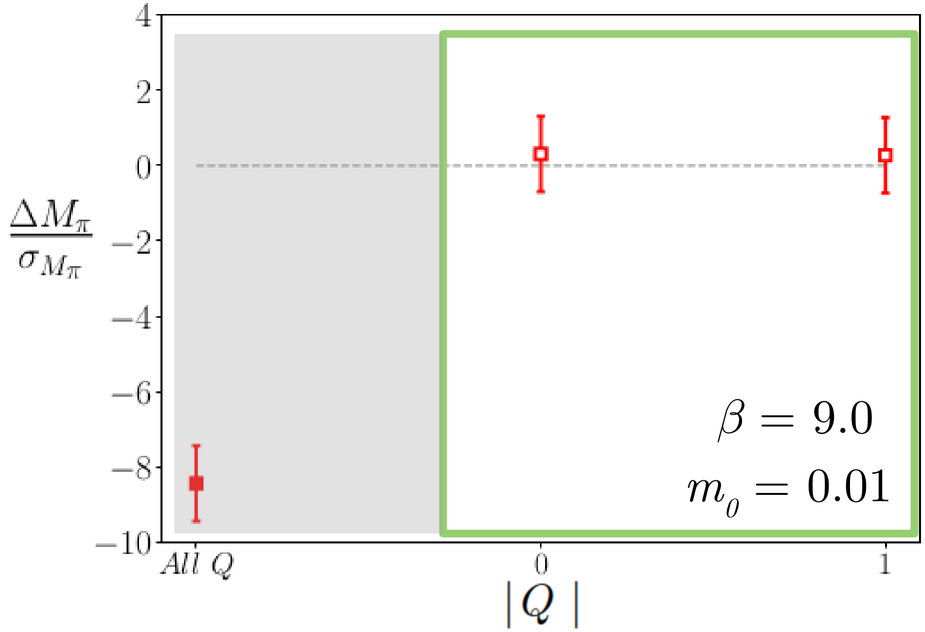


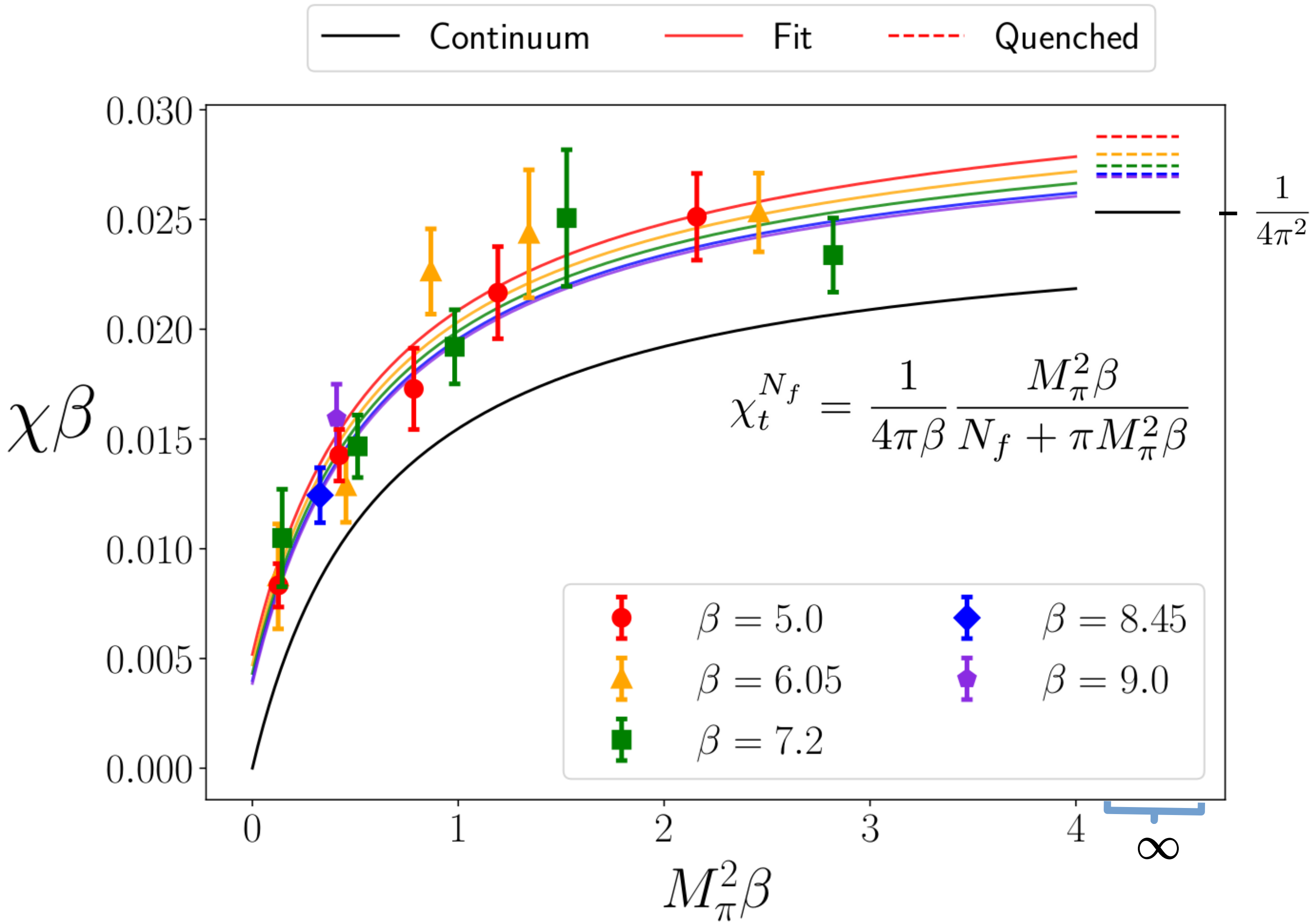
★ HMC has 8σ discrepancy with wHMC in the topological average

Pion Mass discrepancy between wHMC and HMC



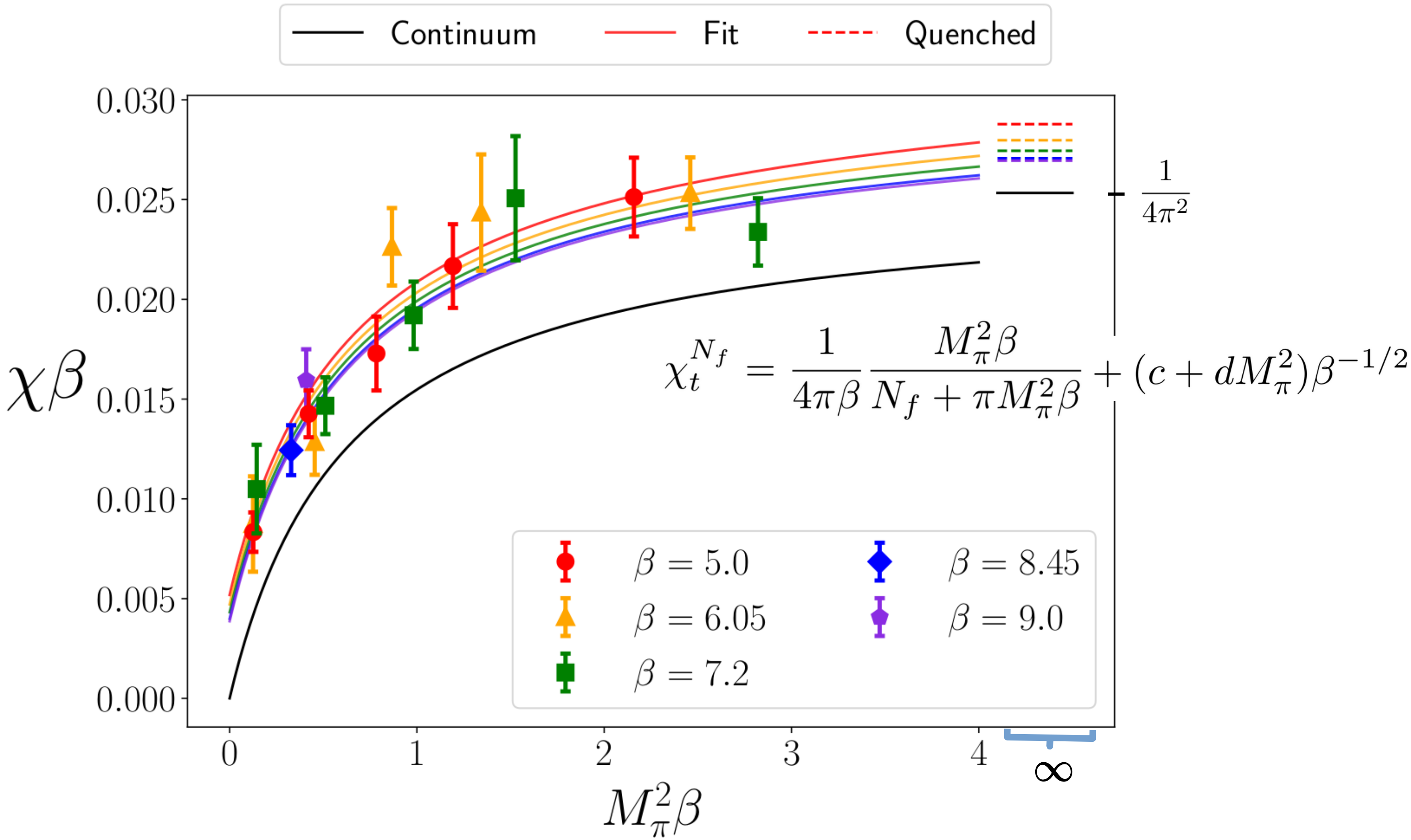
- HMC has 8σ discrepancy with wHMC in the topological average
- but samples correctly $Q = 0$ and $Q = 1$

$N_f = 2$ results



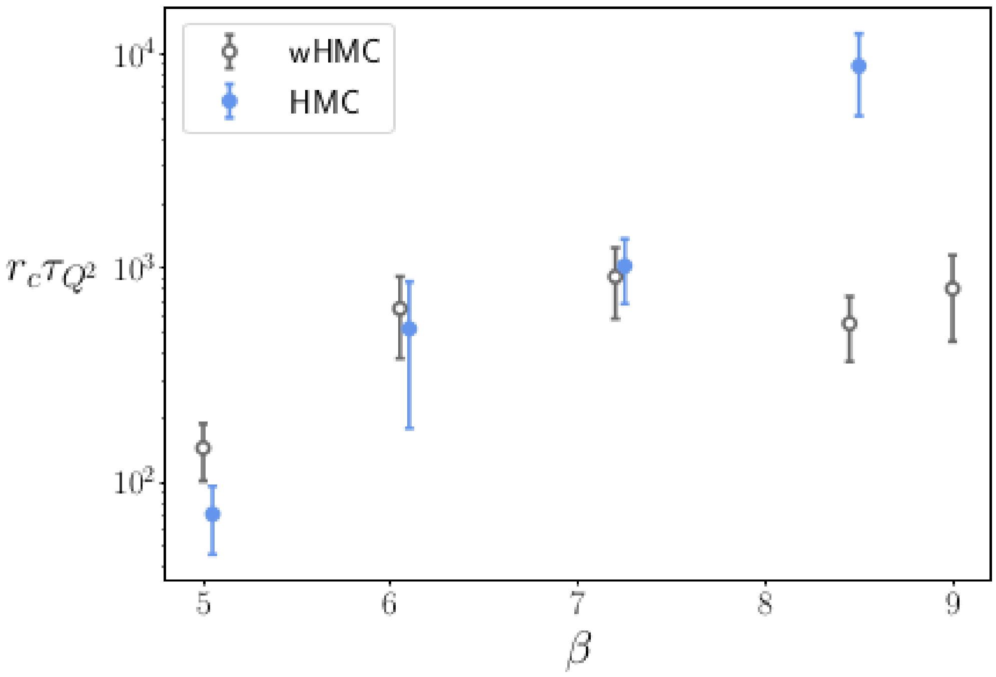
Good agreement with chiral and quenched limits

$N_f = 2$ results



Good agreement with chiral and quenched limits

$N_f = 2$ results: scaling with a



☆ At equivalent computational costs, topology freezing is improved with wHMC with respect to HMC

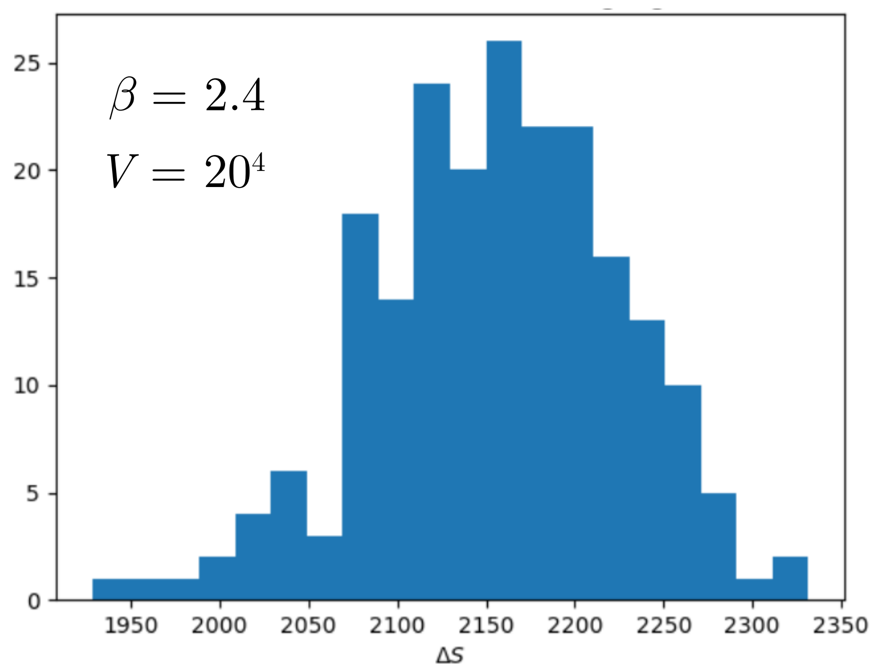
Summary & Outlook

- ☆ We have built an algorithm which improves topological freezing for a U(1) gauge theory with $N_f = 0$ and $N_f = 2$
- ☆ We have seen that HMC is biased in topological (susceptibility) and non-topological (plaquette, pion mass) observables close to the continuum limit
- ☆ We have checked that HMC samples correctly at fixed topology despite being frozen

- ☆ We are exploring the implementation of the algorithm for a SU(2) gauge theory in 4D

Backup

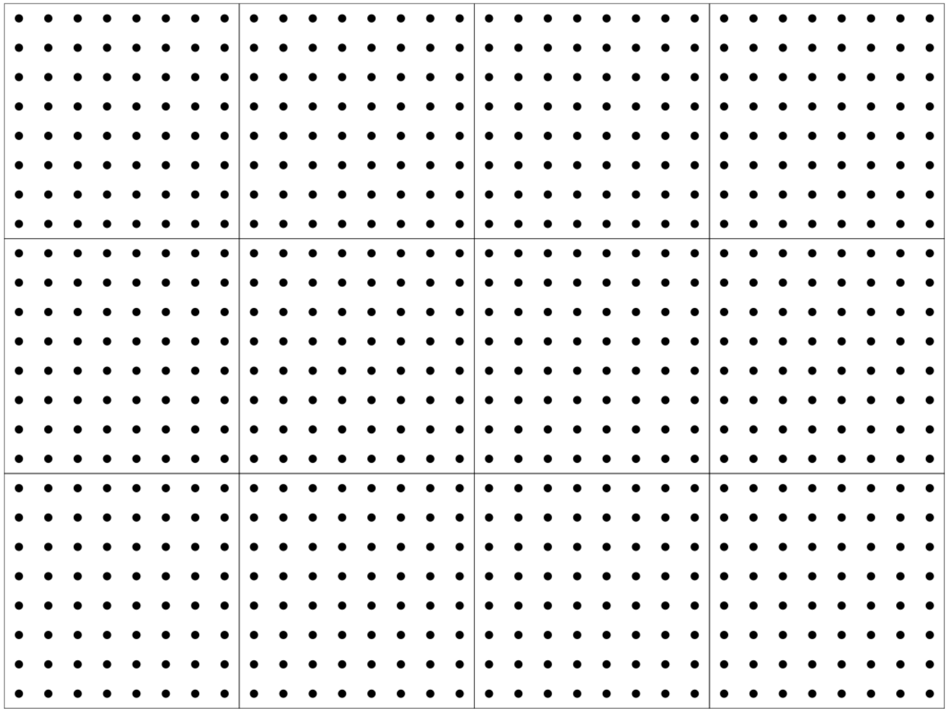
Can wHMC be generalized to 4D?

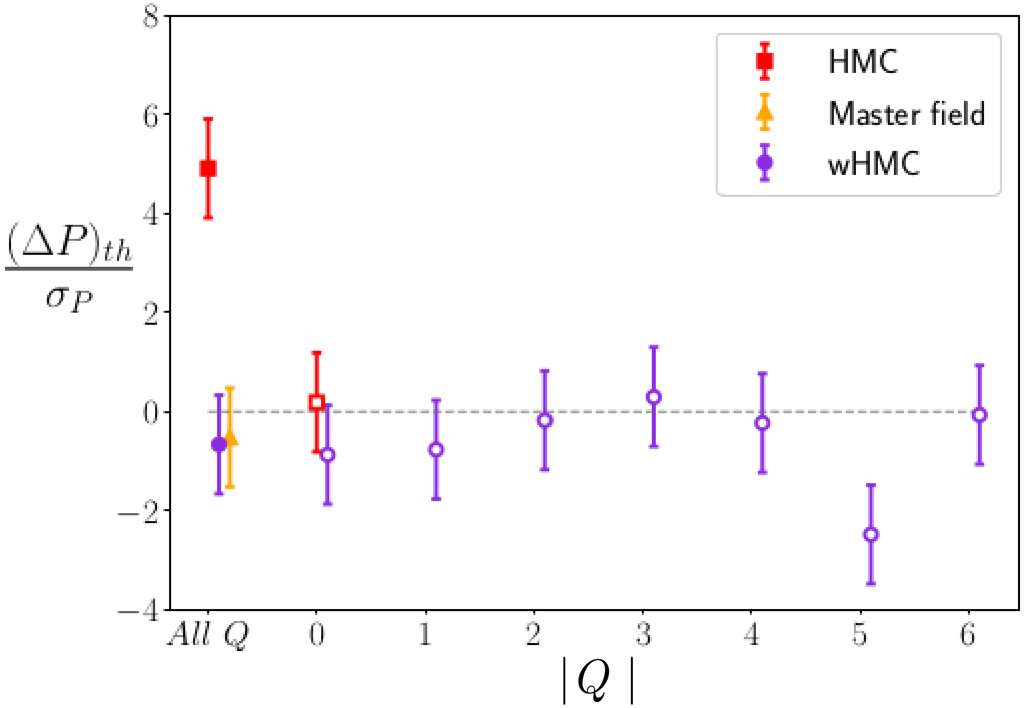


SU(2) gauge theory

- Tried a naive generalization, but acceptances are very low

Master fields

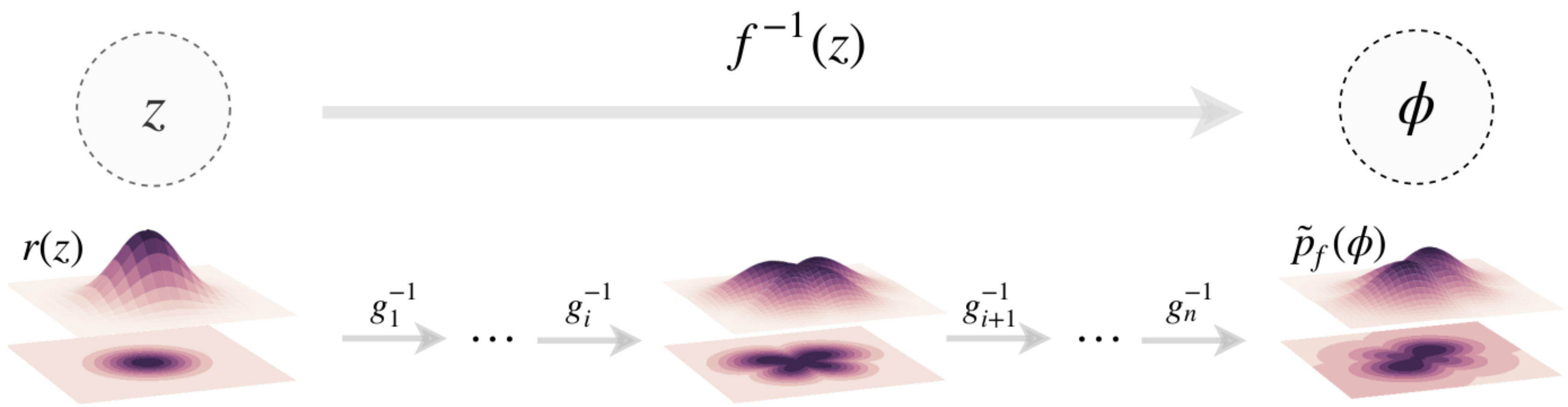




M. Lüscher, EPJ Web Conf. 175, 01002 (2018), 1707.09758.

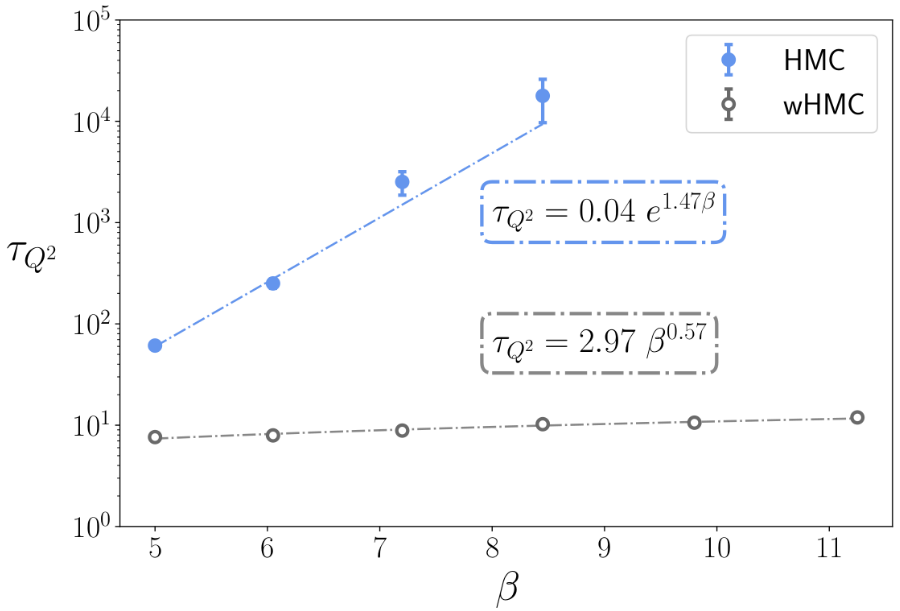
- Perform spacetime averages in huge lattices instead of Monte-Carlo-time averages
- Does not suffer from topology freezing
- Can extract observables from one single configuration, but hard to thermalize!

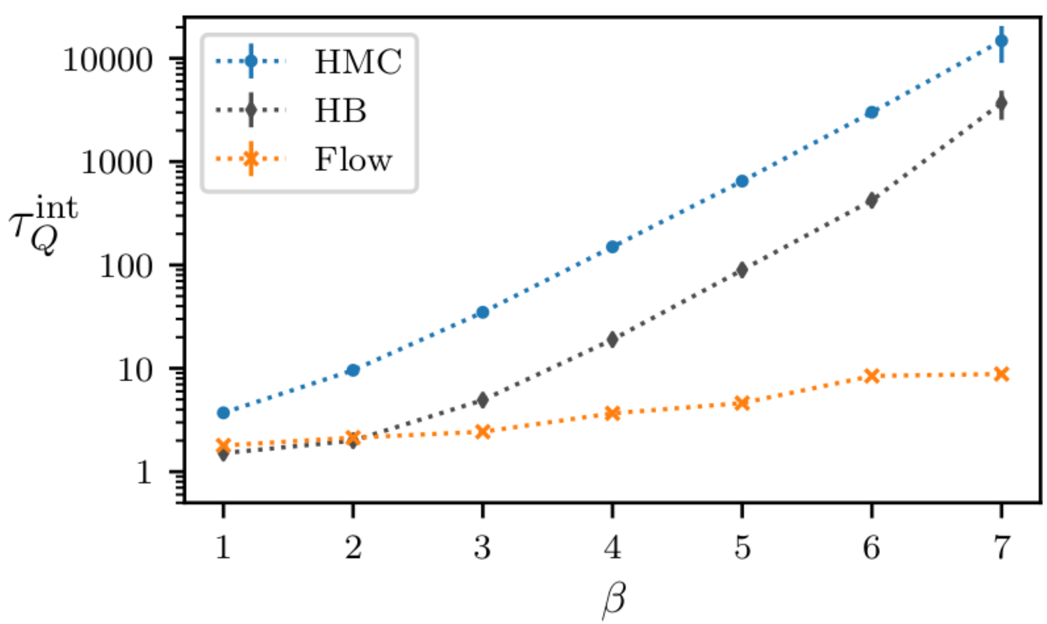
Equivariant flow-based sampling in U(1)



(a) Normalizing flow between prior and output distributions

M. S. Albergo, G. Kanwar and P. E. Shanahan, Phys. Rev. D 100, 034515 (2019), 1904.12072





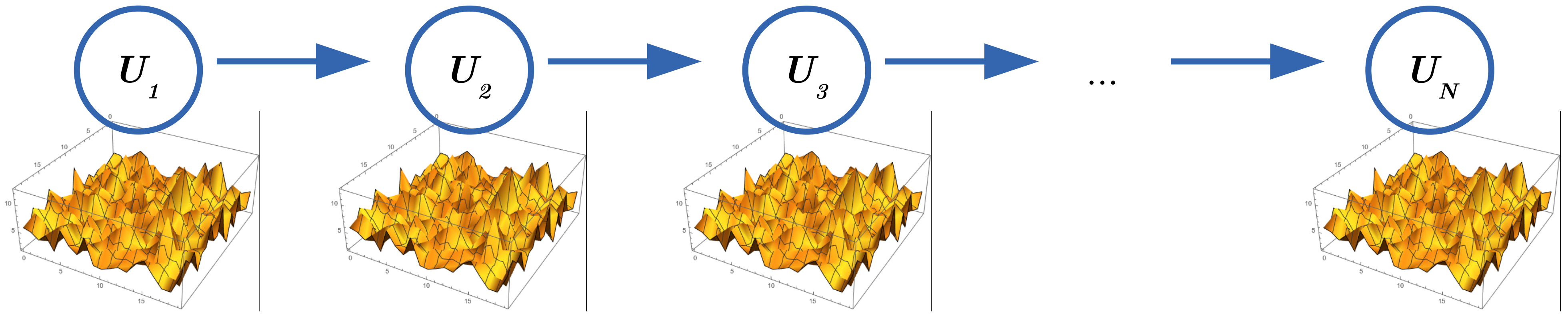
G. Kanwar et al., Phys. Rev. Lett. 125, 121601 (2020), 2003.06413

Lattice computations

Expectation value of O : $$\langle O \rangle = \frac{\int DU \;\; O[U] e^{-S[U]}}{\int DU e^{-S[U]}}$$ U : gauge links

Usual workflow in lattice computations

1. Interpret $e^{-S[U]}$ as a probability distribution
2. Generate N configurations following $e^{-S[U]}$ using Hybrid Monte Carlo (HMC)



3. Extract observables of interest by averaging over the generated configurations

$$\langle O \rangle = \frac{1}{N} \sum_{i=1}^{N} O(\{U\}_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$