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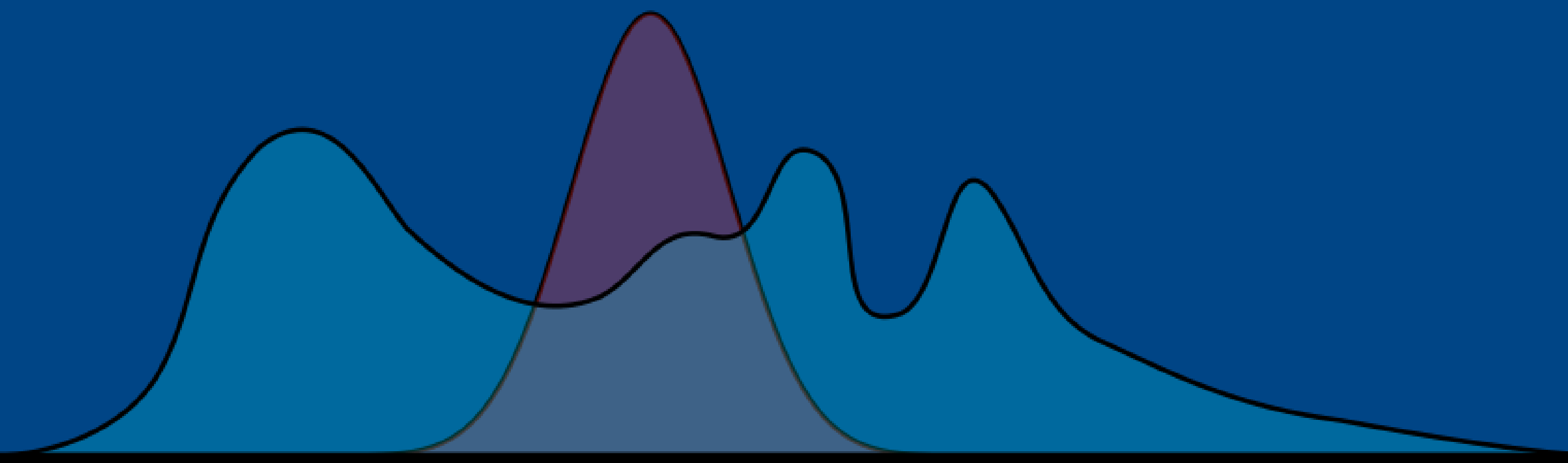

Improved topological sampling for lattice gauge theories

David Albandea

HU Berlin / NIC DESY Zeuthen Lattice Seminar

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)

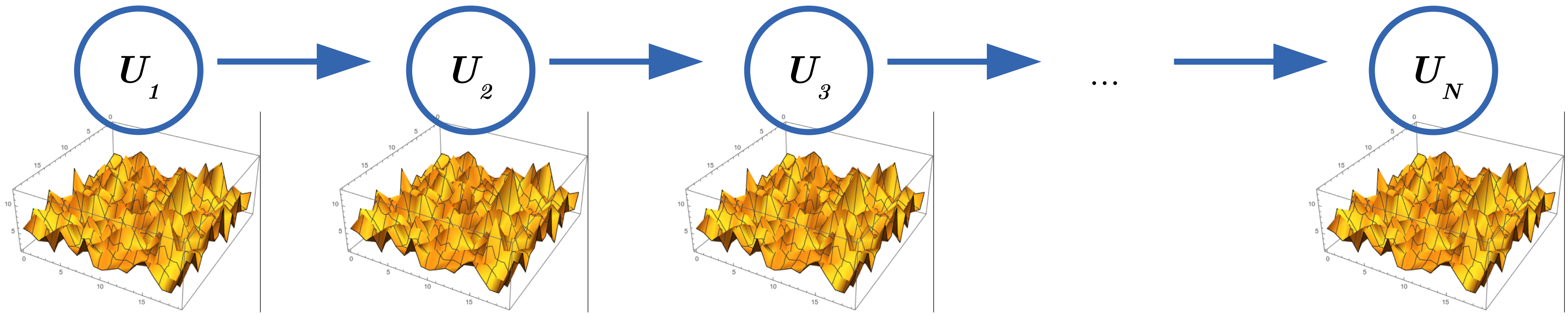
We propose a modification of the Hybrid Monte Carlo (HMC) algorithm that overcomes the topological freezing of a two-dimensional $U(1)$ gauge theory with and without fermion content. This algorithm includes reversible jumps between topological sectors—winding steps—combined with standard HMC steps. The 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 $L \sim 8 \times 10^3$.

Lattice computations

Expectation value of O : $$\langle O \rangle = \frac{1}{Z} \int DU \, O(U) e^{-S(U)}$$ 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

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

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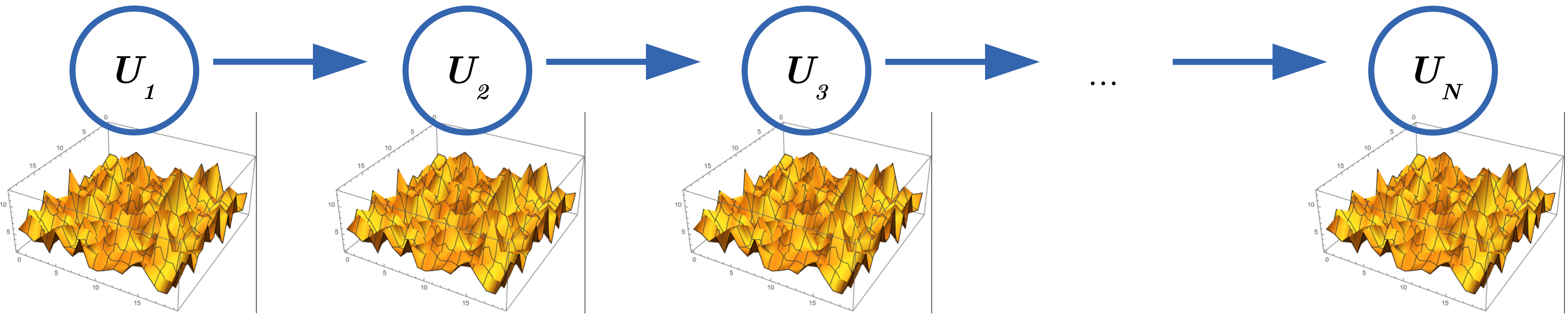

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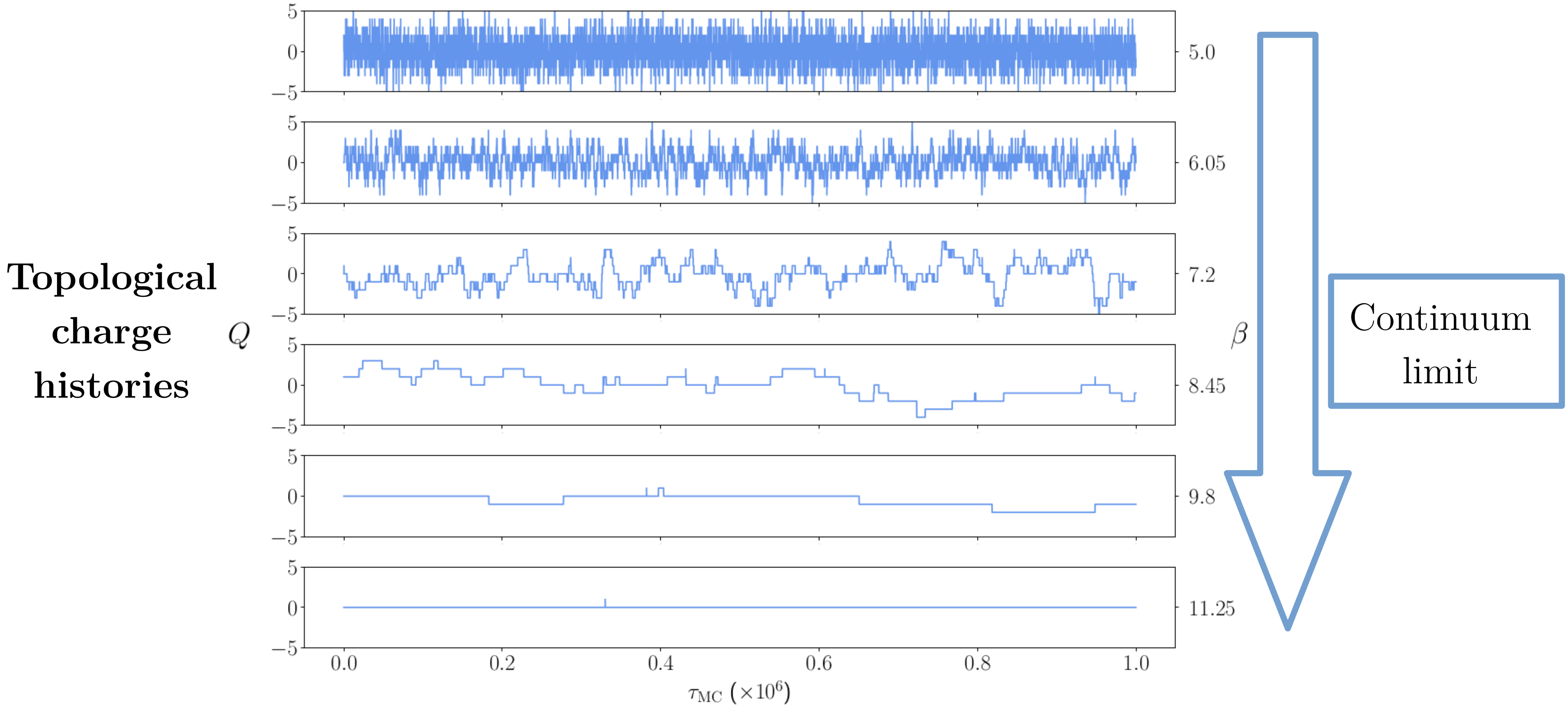
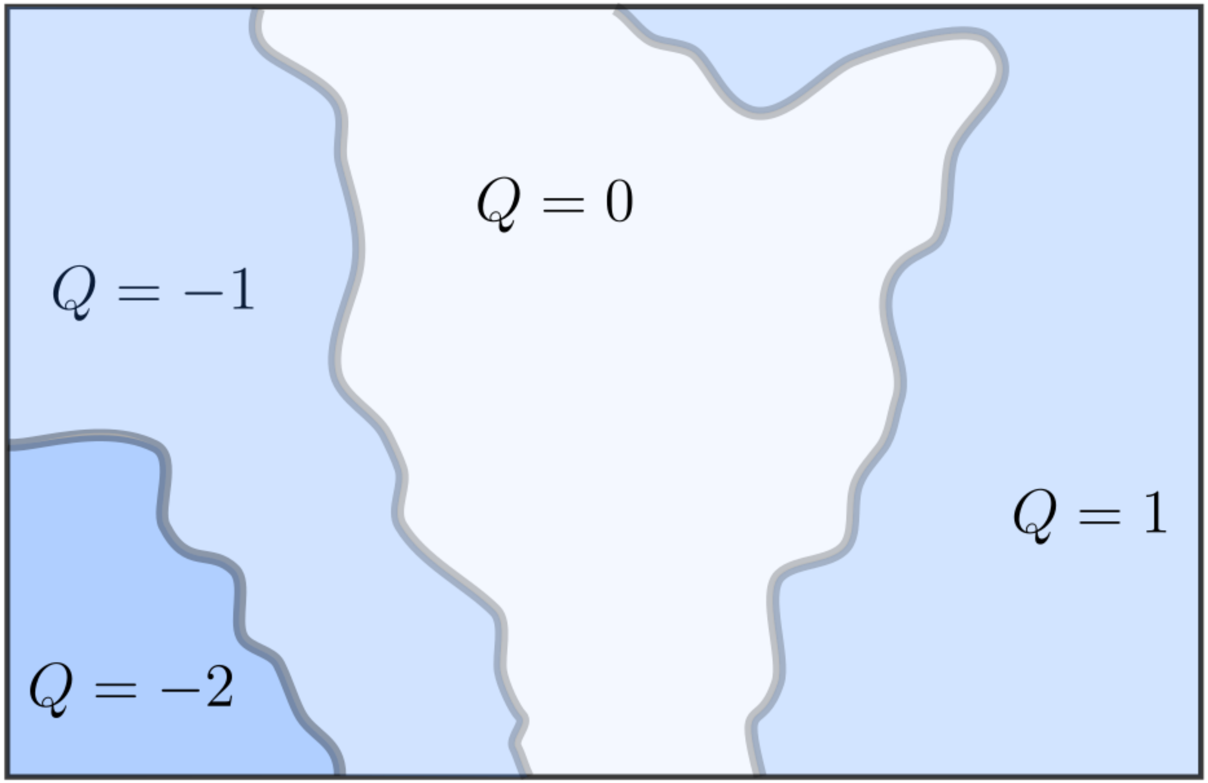


☆ Topological charge freezes going to the continuum

⇨ **Long autocorrelation times**

Topology freezing



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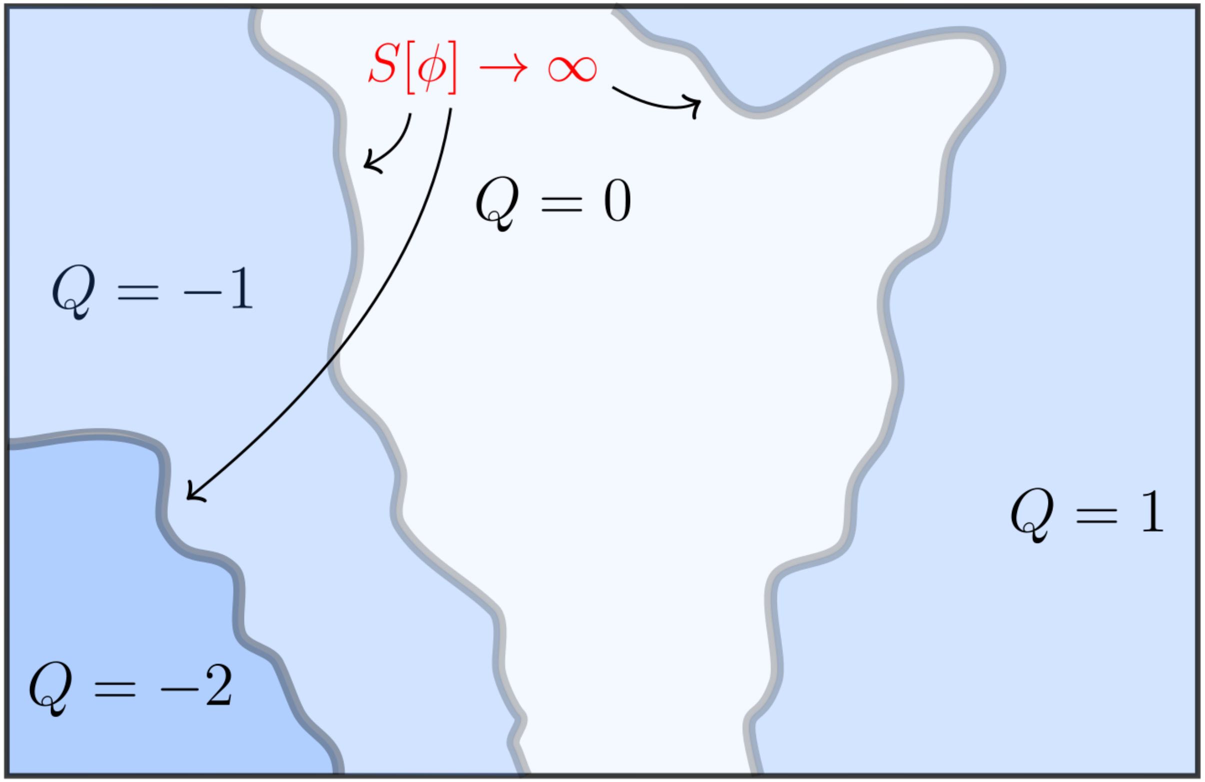

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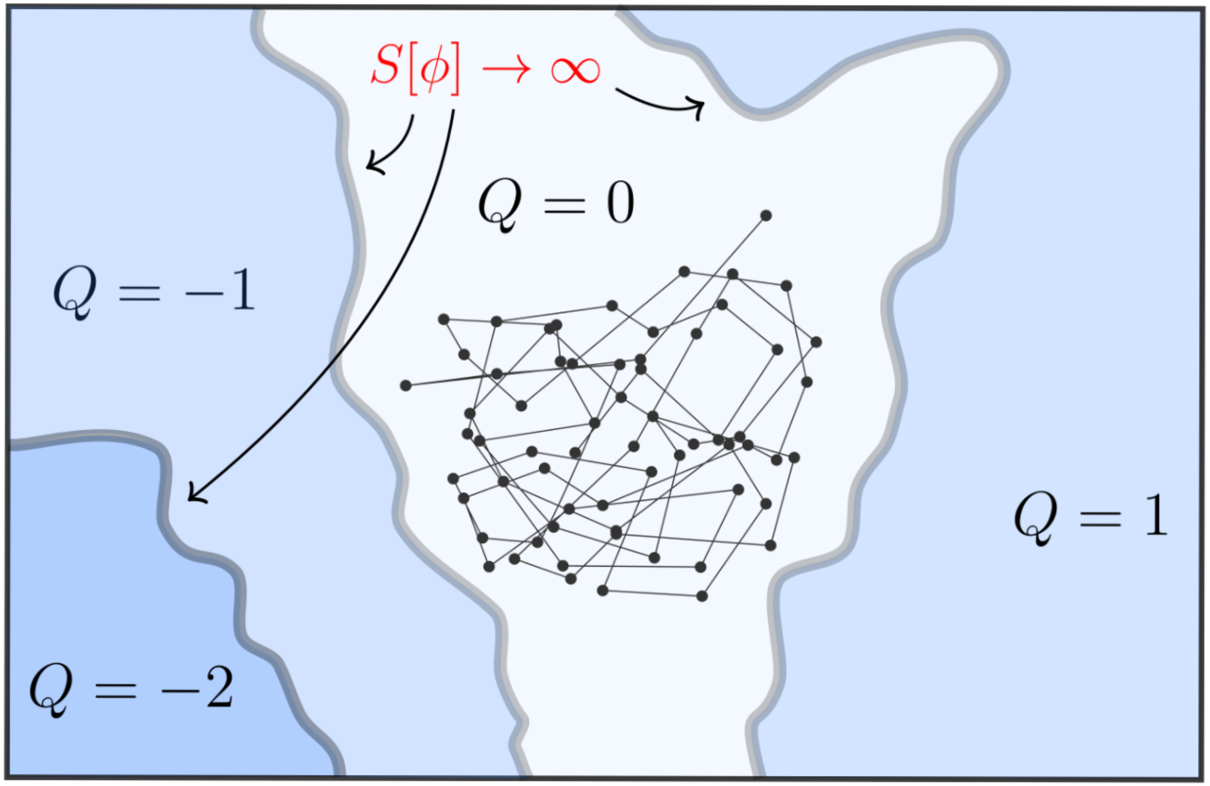

- HMC proposes configurations with the same Q

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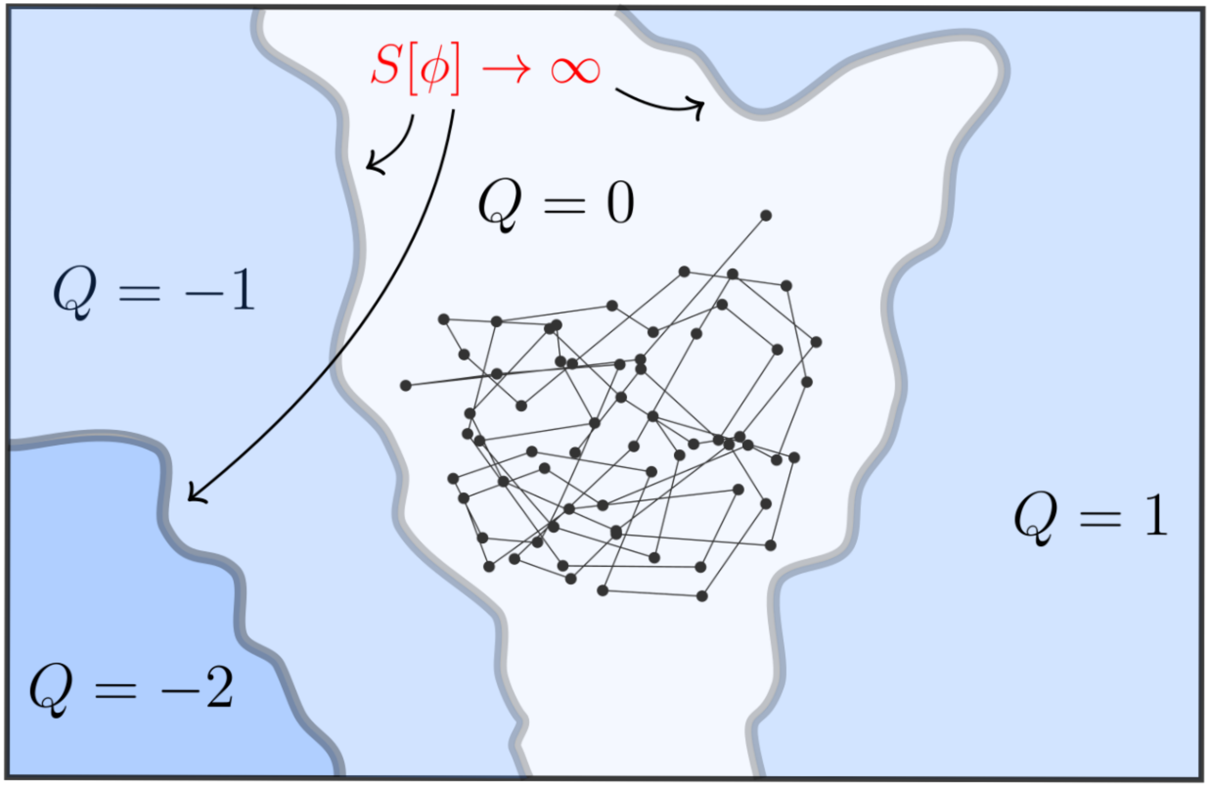

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Can we build an algorithm that proposes

$$Q \to Q \pm 1$$

more frequently than HMC?

The model

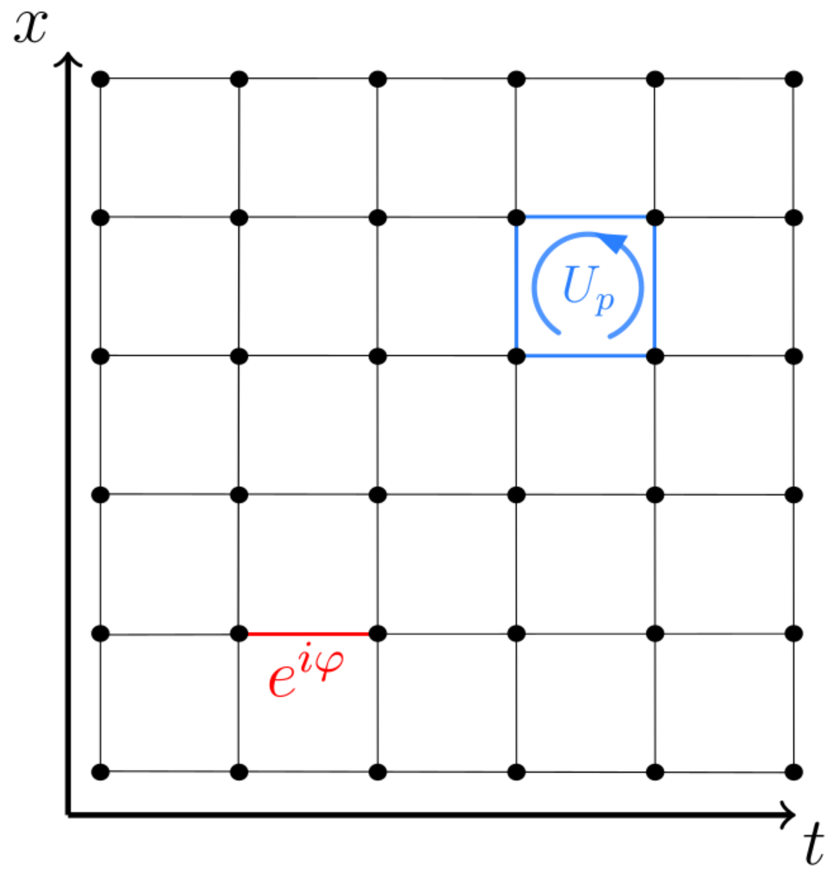
- We worked in U(1) gauge theory in 2D for $N_f = 0$ and $N_f = 2$
  - used as benchmark model in Machine Learning, Tensor Networks...

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

Nice features:

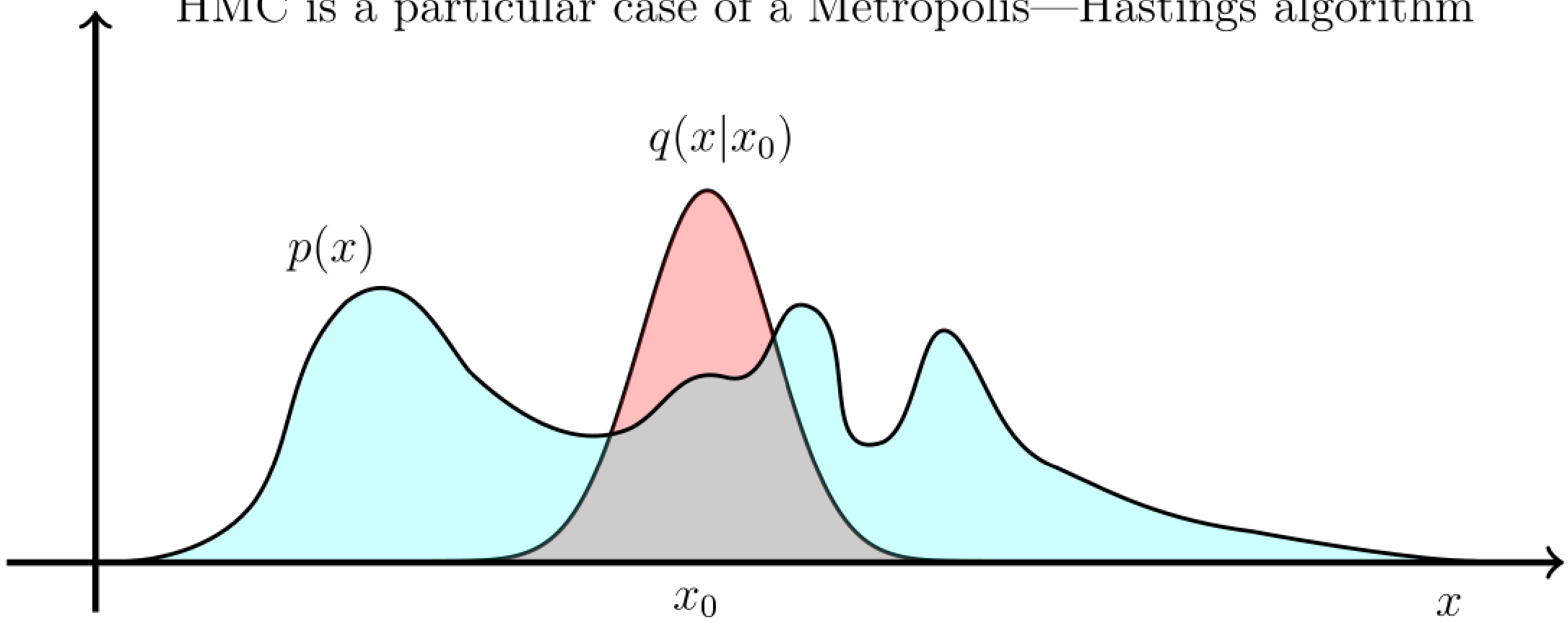
- It is similar to QCD
  - Topology
  - Mass gap ($N_f = 2$)
- Analytical results for $N_f = 0$ at finite β and V
- Topological charge is exactly an integer

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



Hybrid Monte Carlo

HMC is a particular case of a Metropolis—Hastings algorithm



Target distribution

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

Proposal distribution

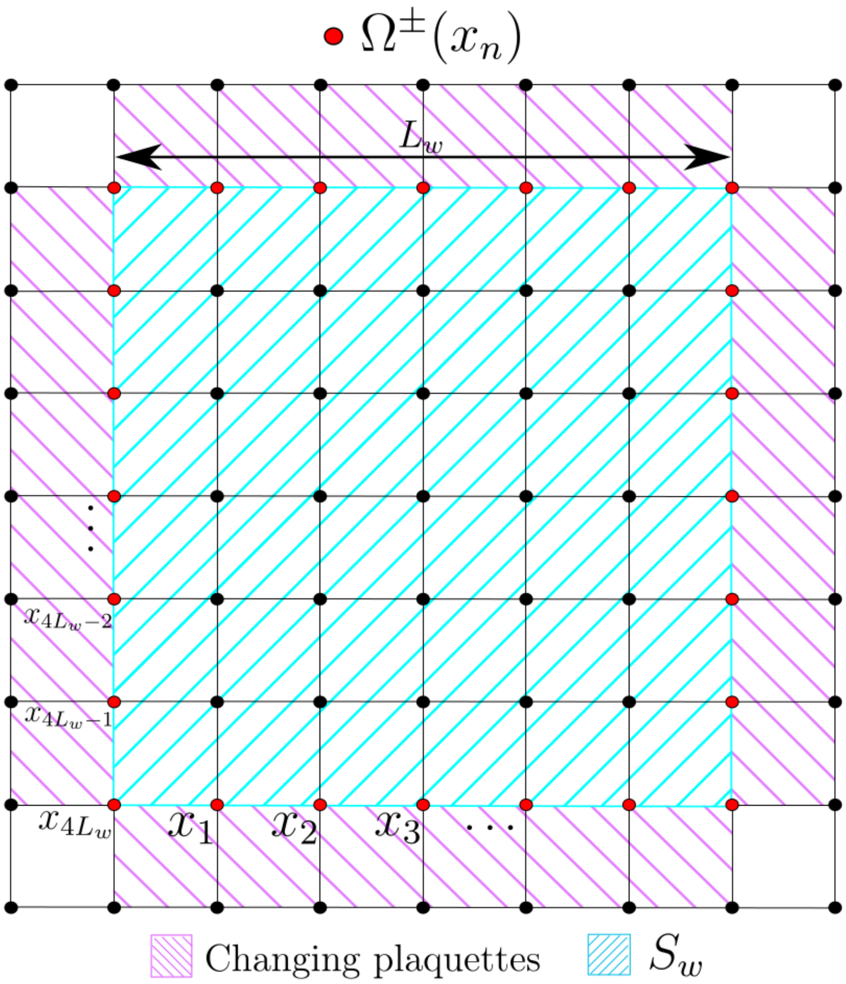
$$q(x'|x) \rightarrow \text{Hamilton eqs.}$$

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

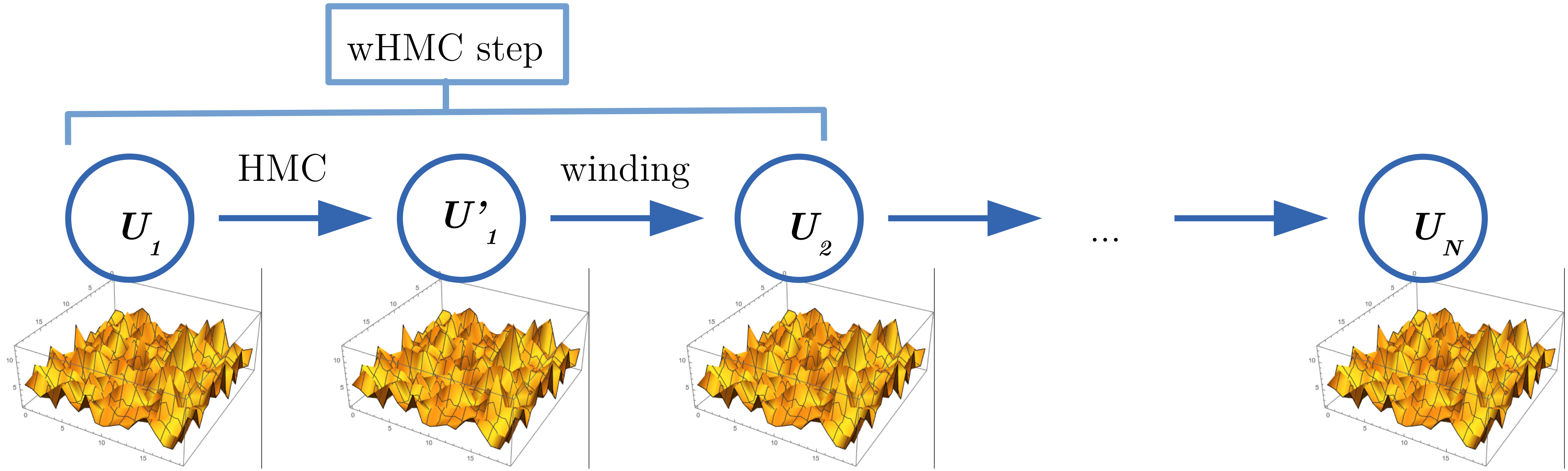
After this, the topological charge is expected to change in one unit

$$Q \to Q \pm 1$$

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

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



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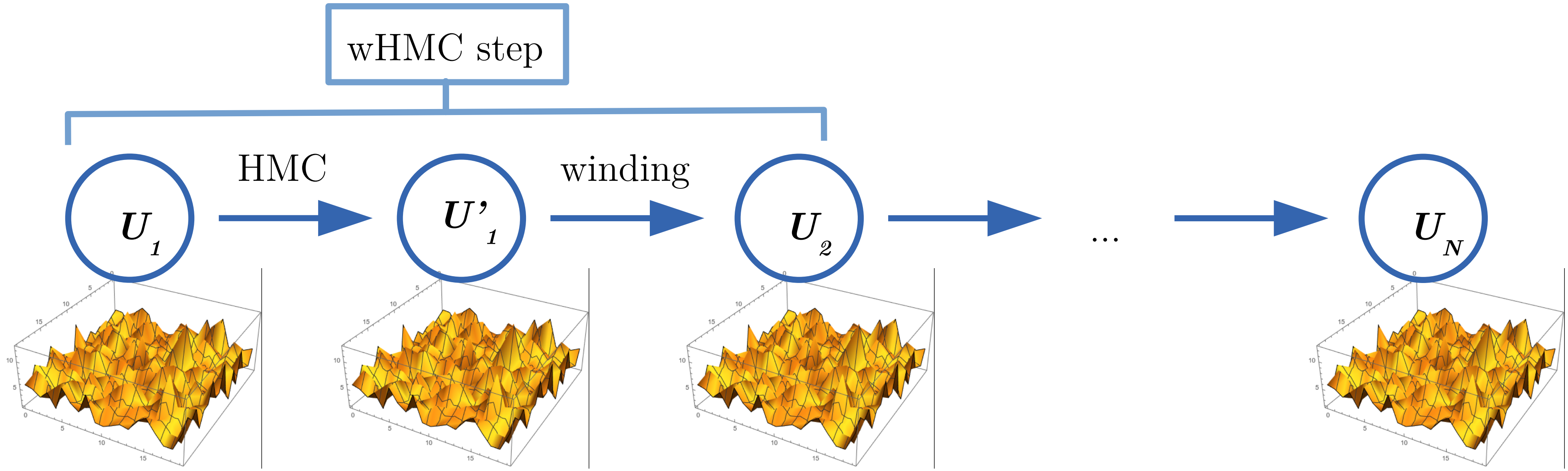
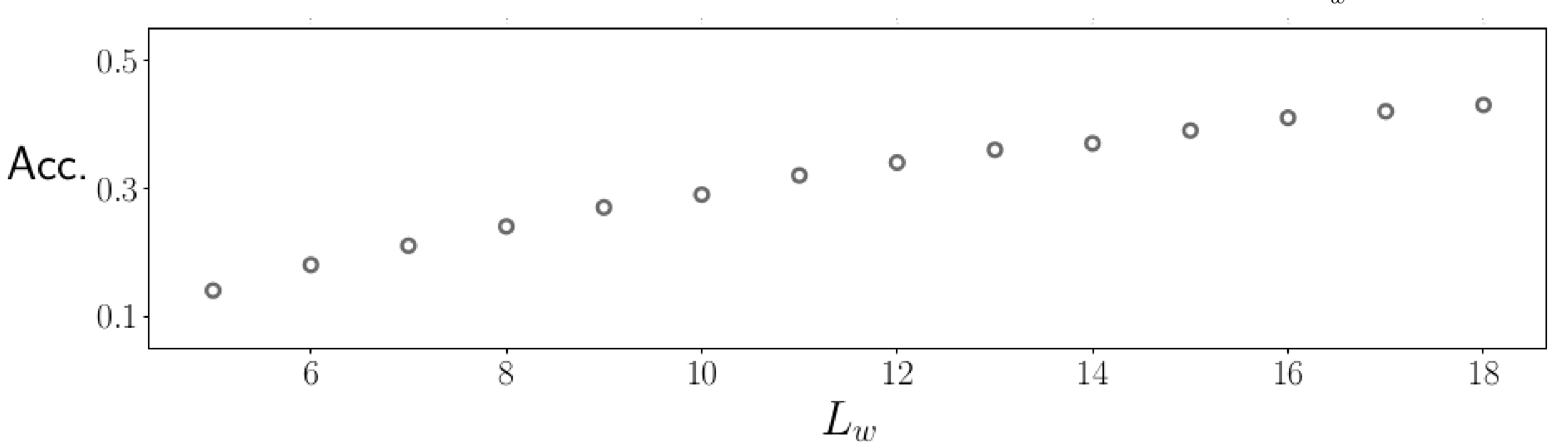


- How does the acceptance of the algorithm change with the size of the winding L_w?

For $N_f = 0$:

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



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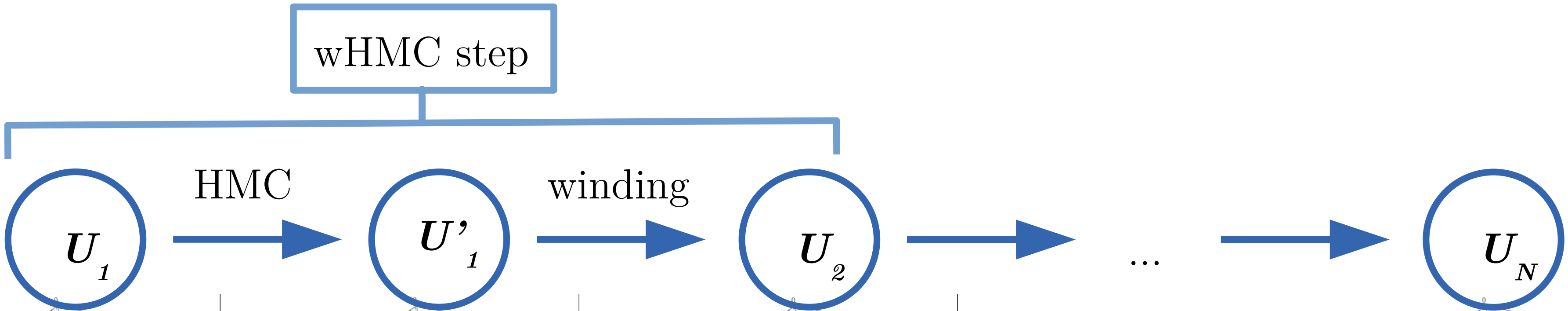

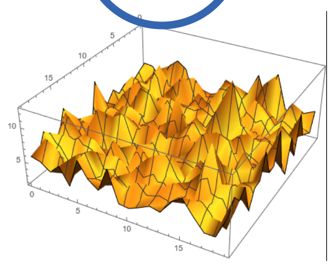

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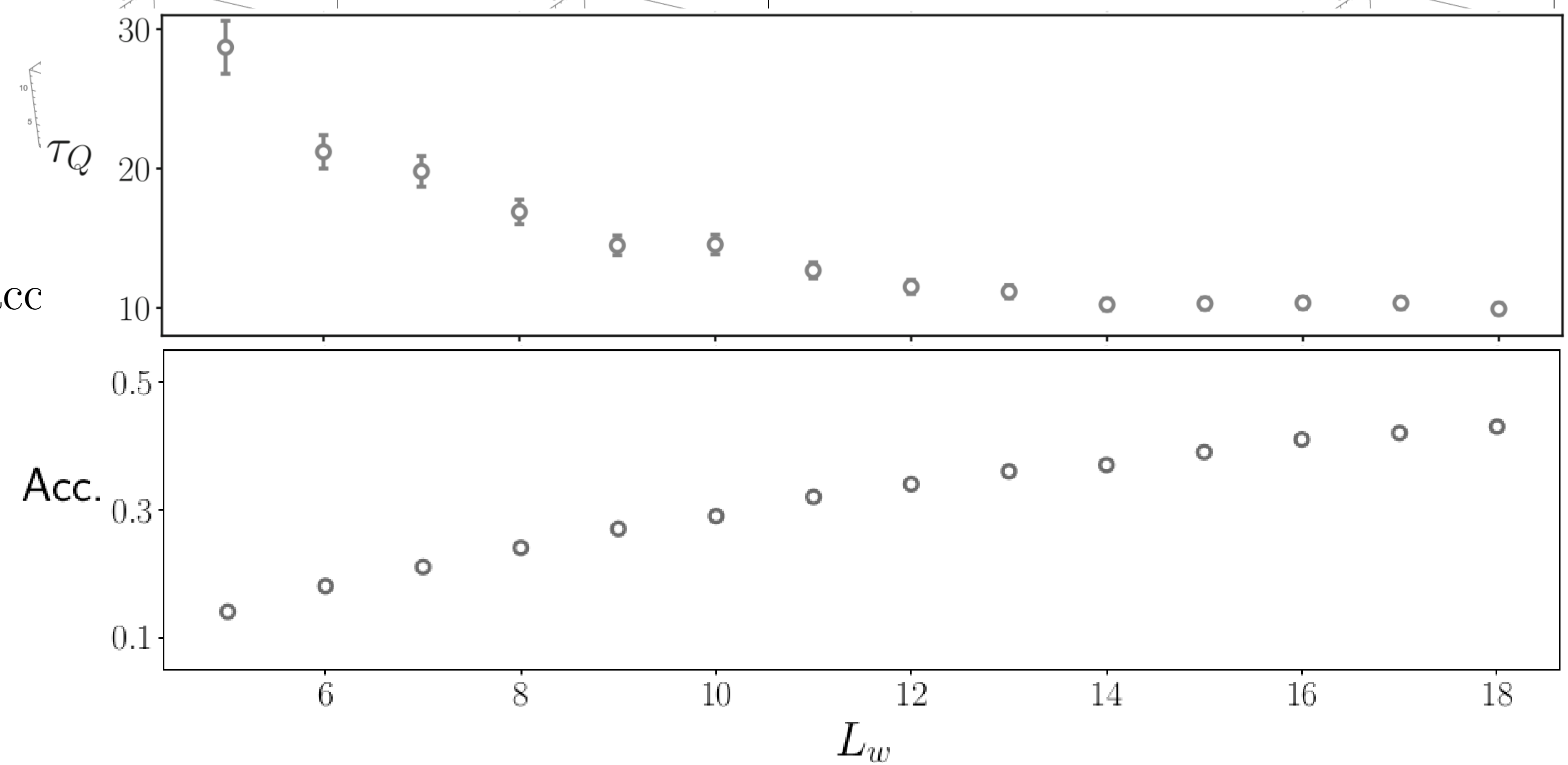
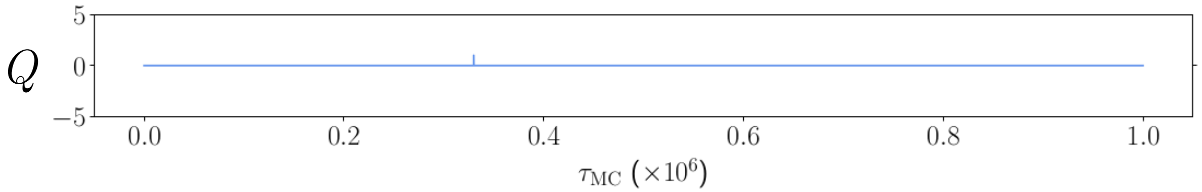
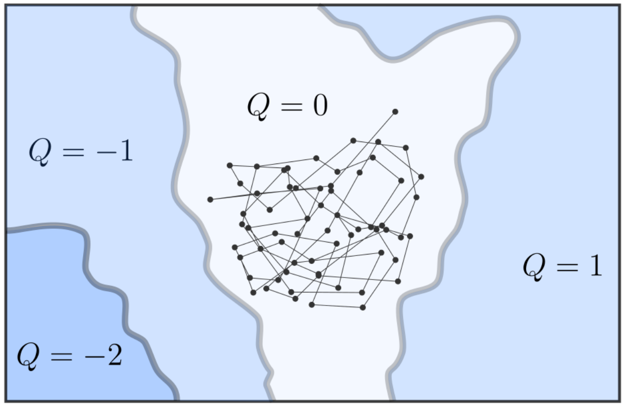


☆ HMC gets stuck in a topological sector Q when approaching the continuum limit, $a \to 0$





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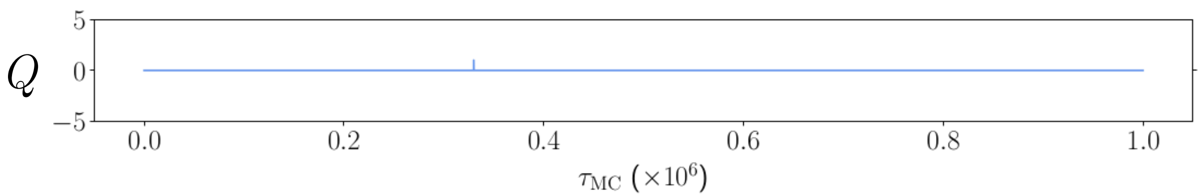
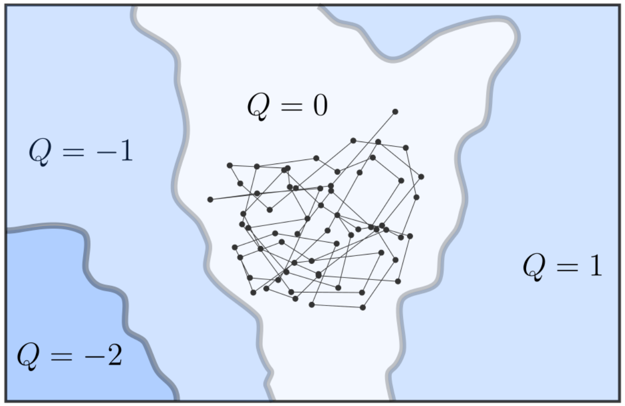
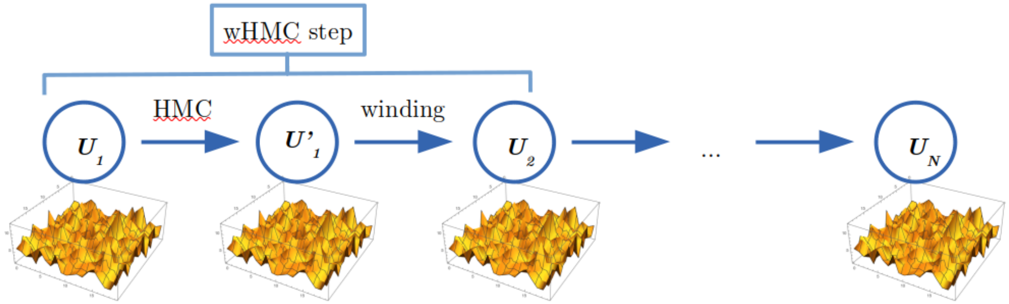
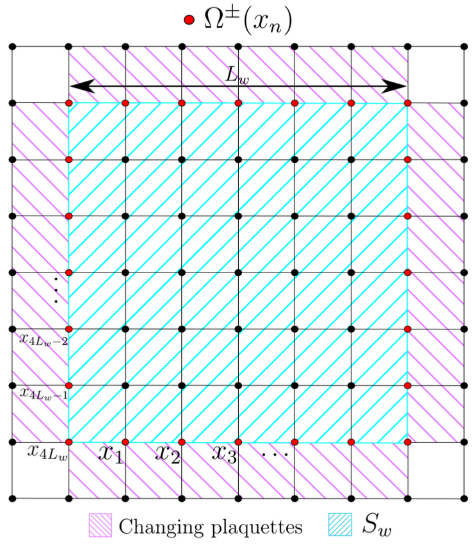




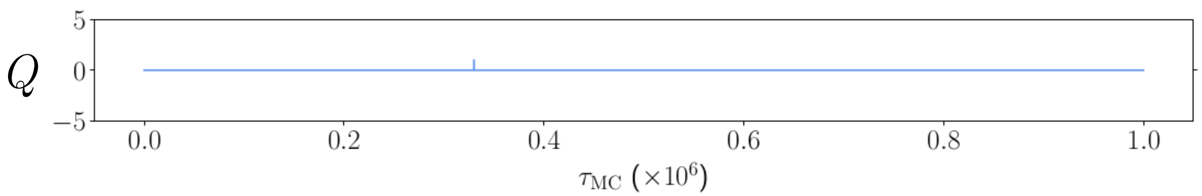
- We have modified HMC with an additional "winding" step that triggers jumps to a different topological sector

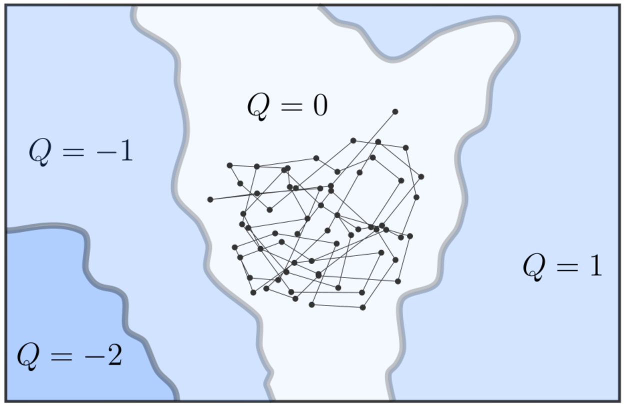




Recap

- HMC gets stuck in a topological sector Q when approaching the continuum limit, $a \to 0$





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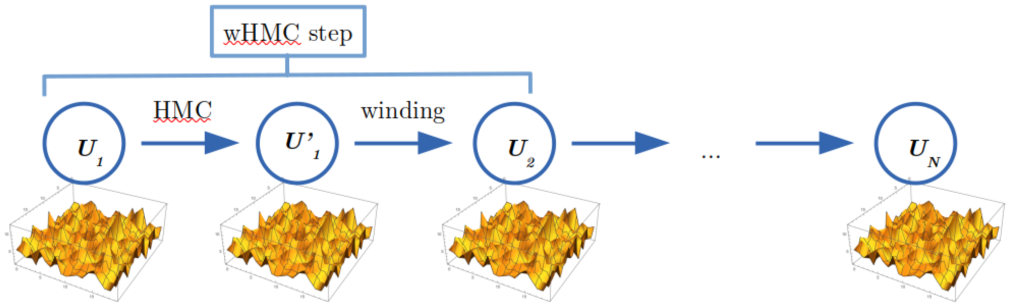
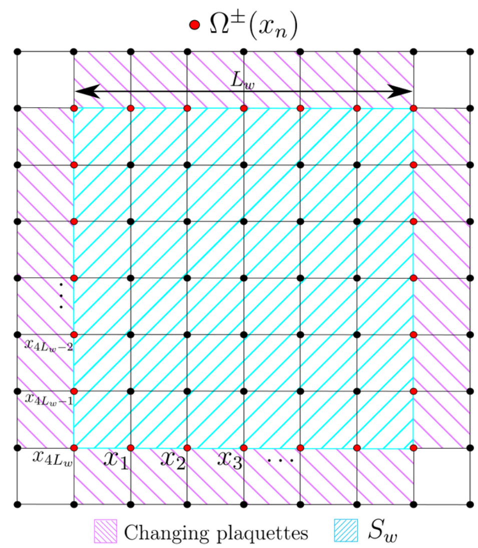
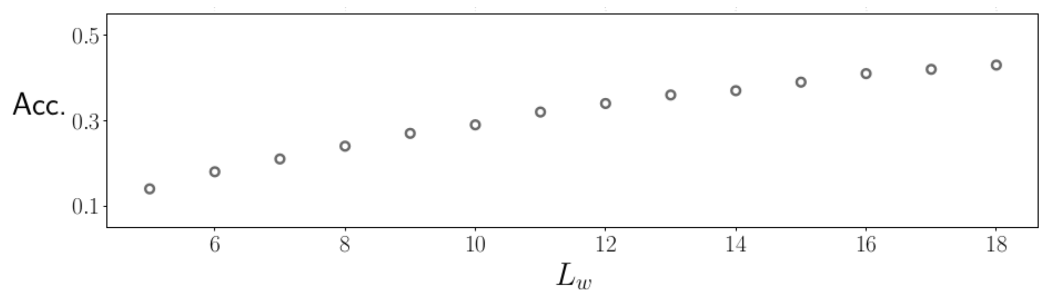




- Without fermions the new algorithm wHMC has acceptance and it increases with the size of the winding



Remaining contents

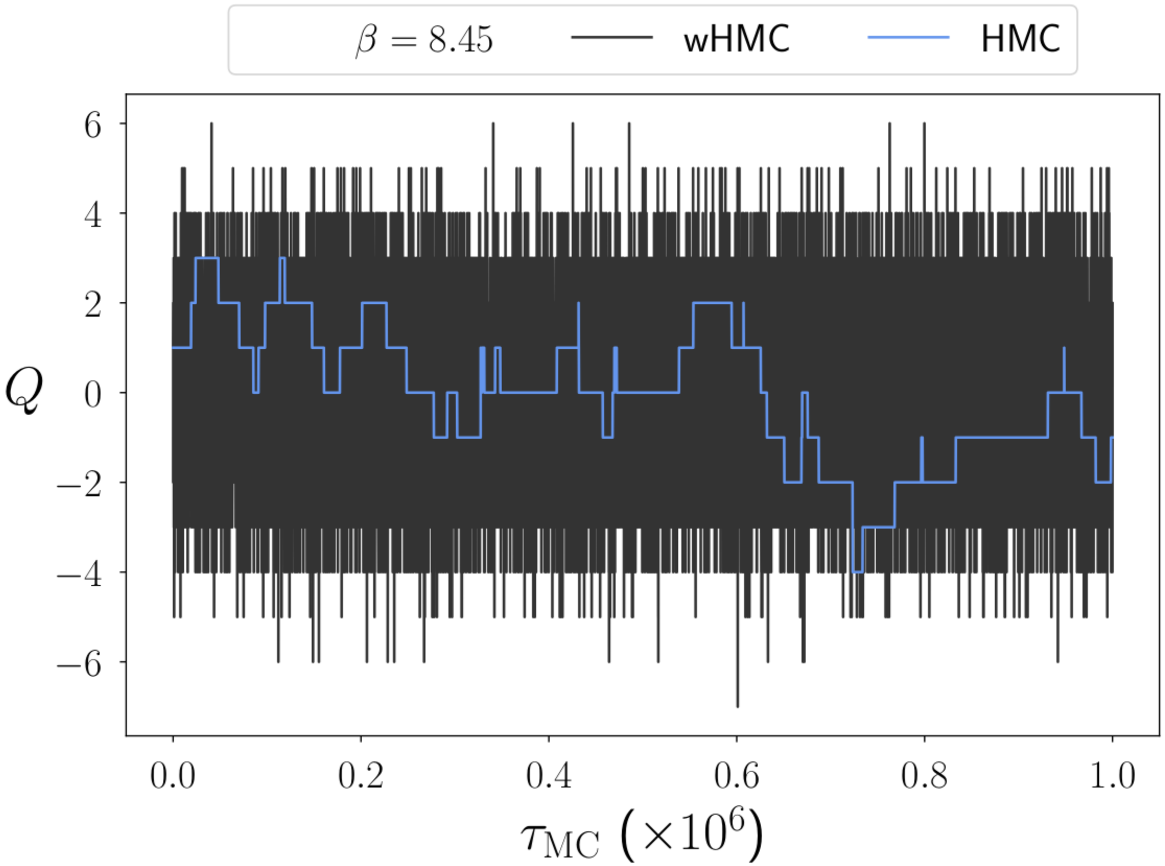
Comparison HMC – wHMC for:

- $N_f = 0$ pure gauge

  ft. Master field simulations

- $N_f = 2$

$N_f = 0$ results



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

⇨ wHMC should lead to correct results

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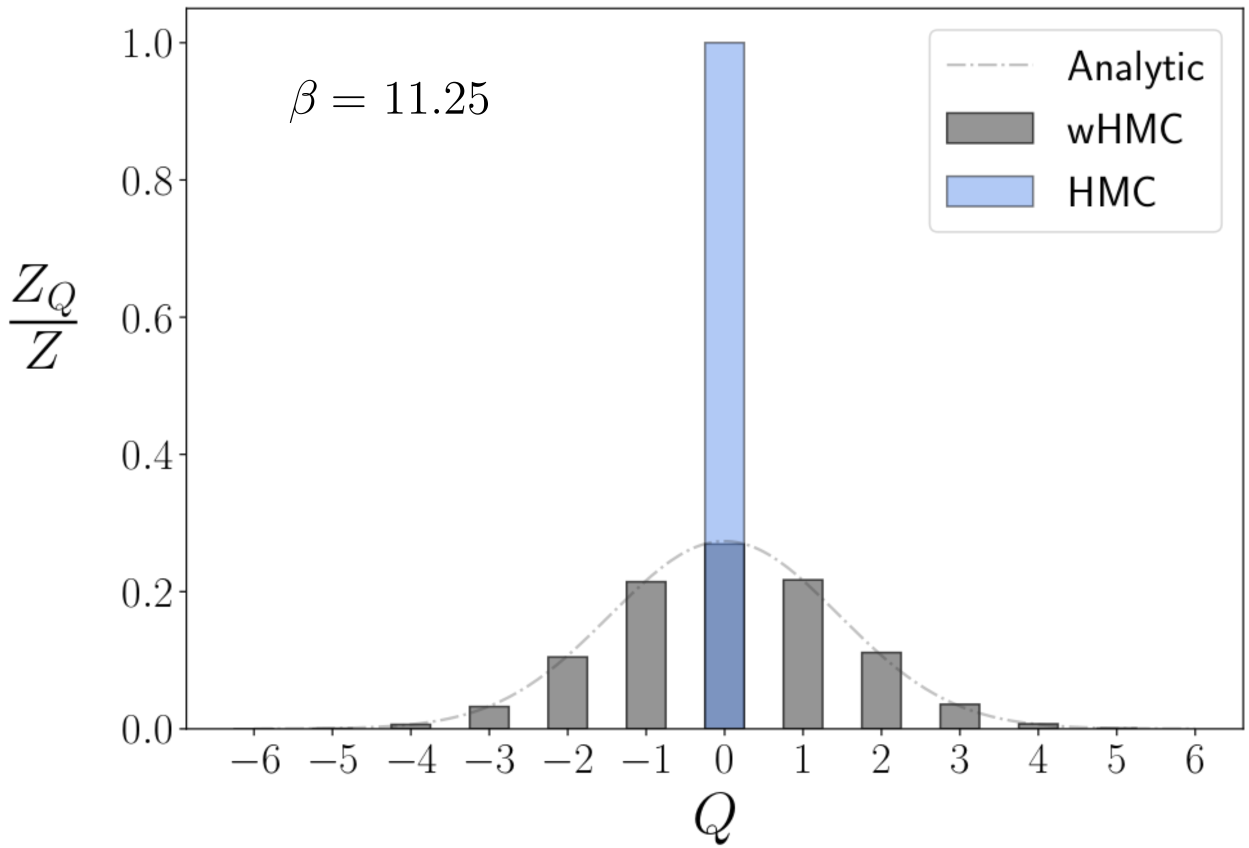
$N_f = 0$ results



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

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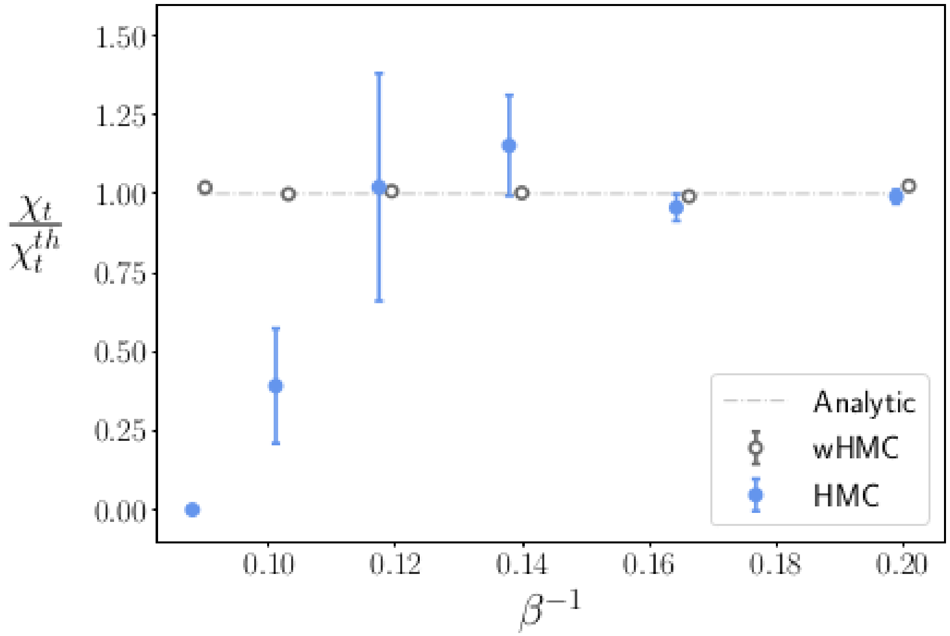
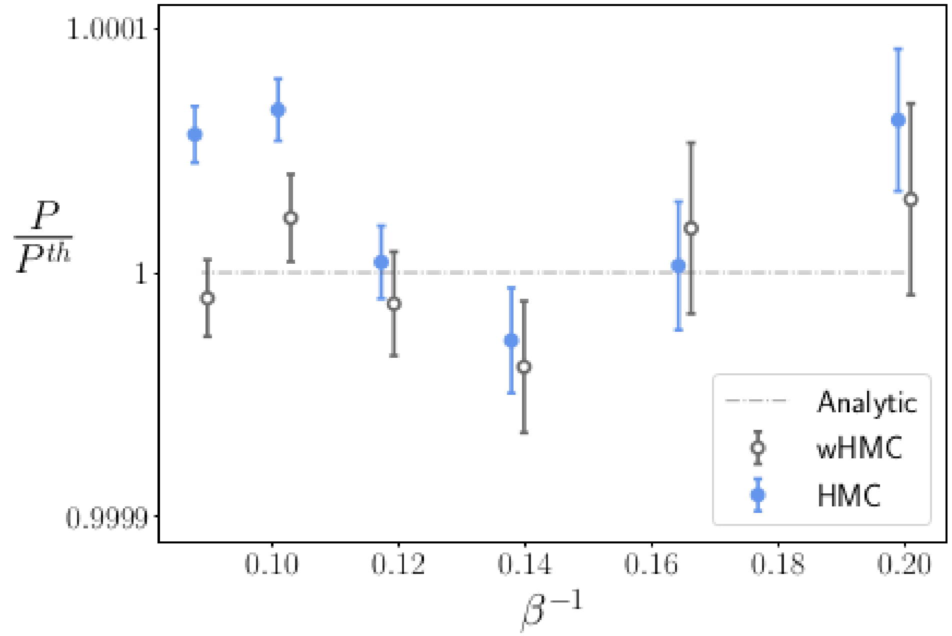
Topological susceptibility



Plaquette



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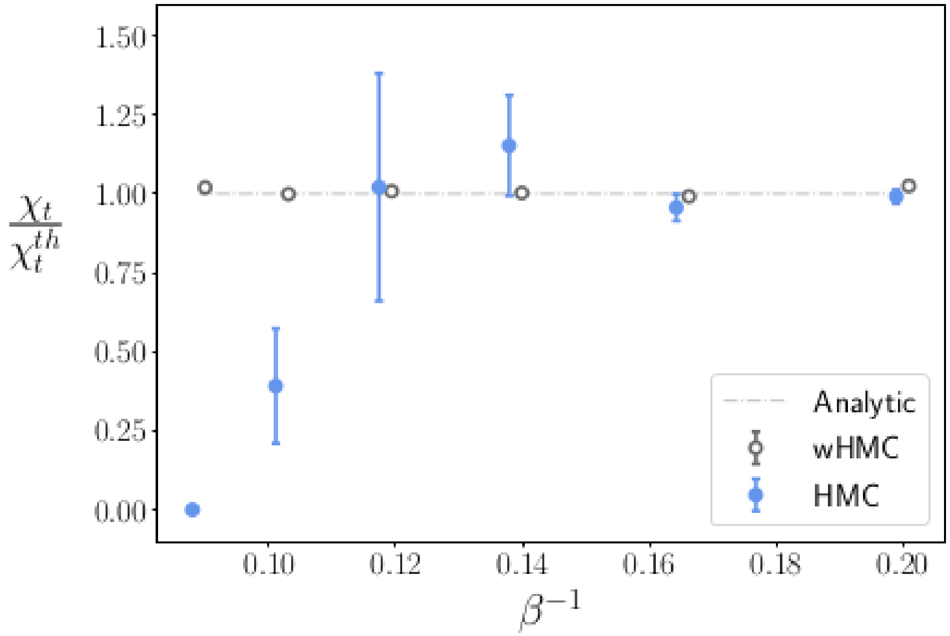

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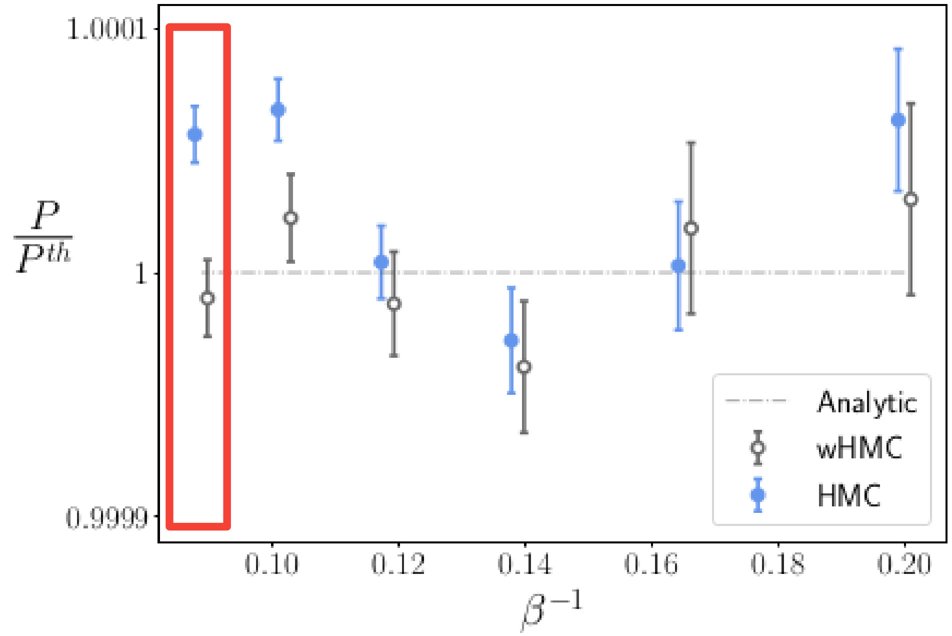

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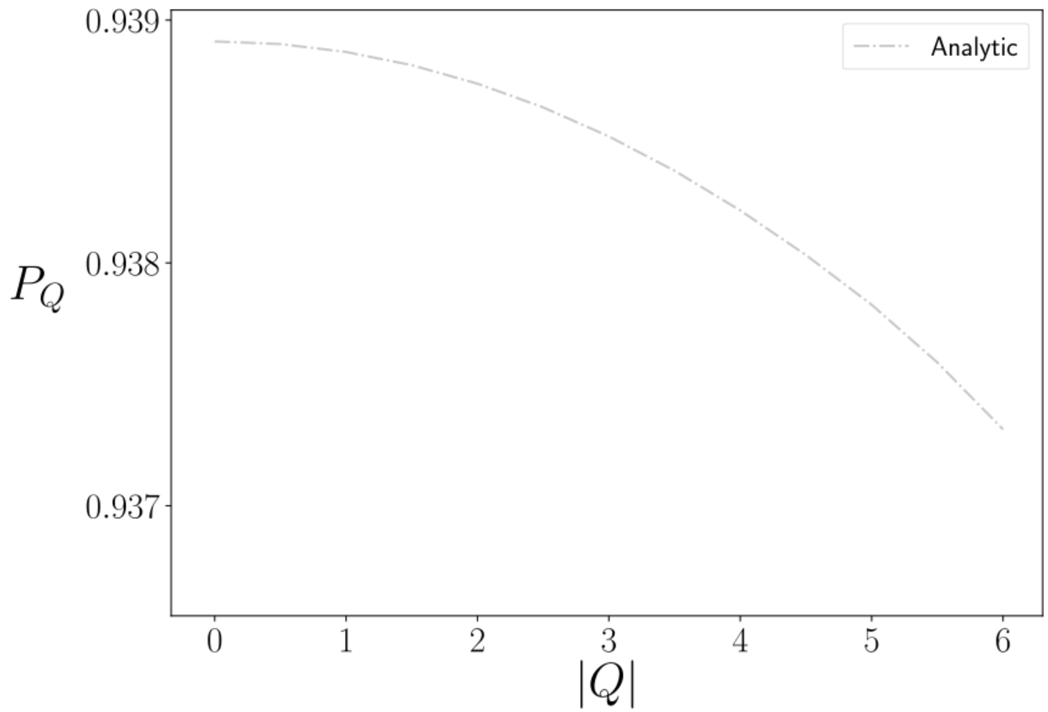

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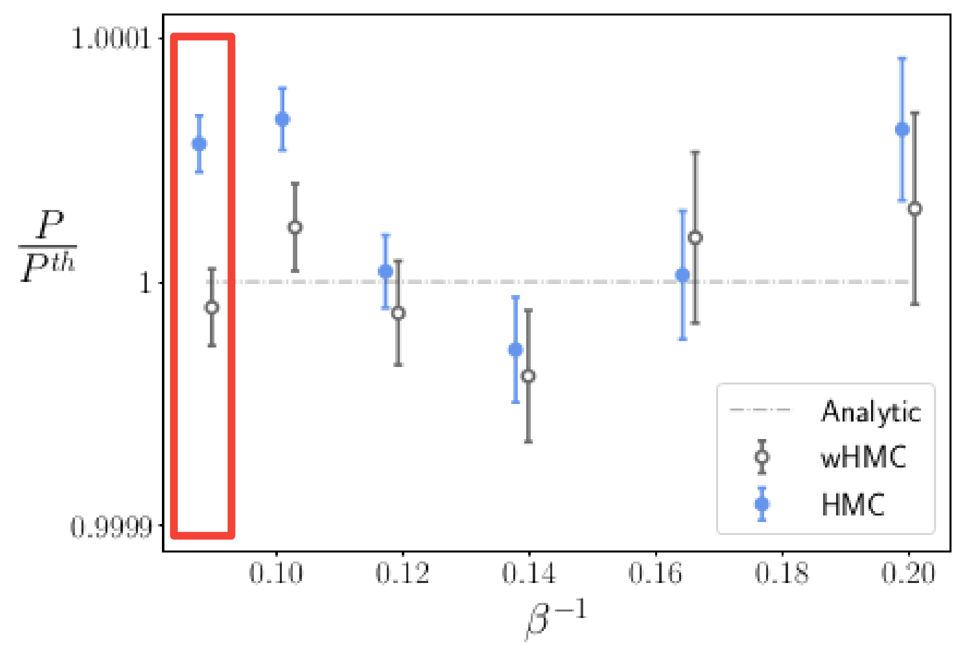

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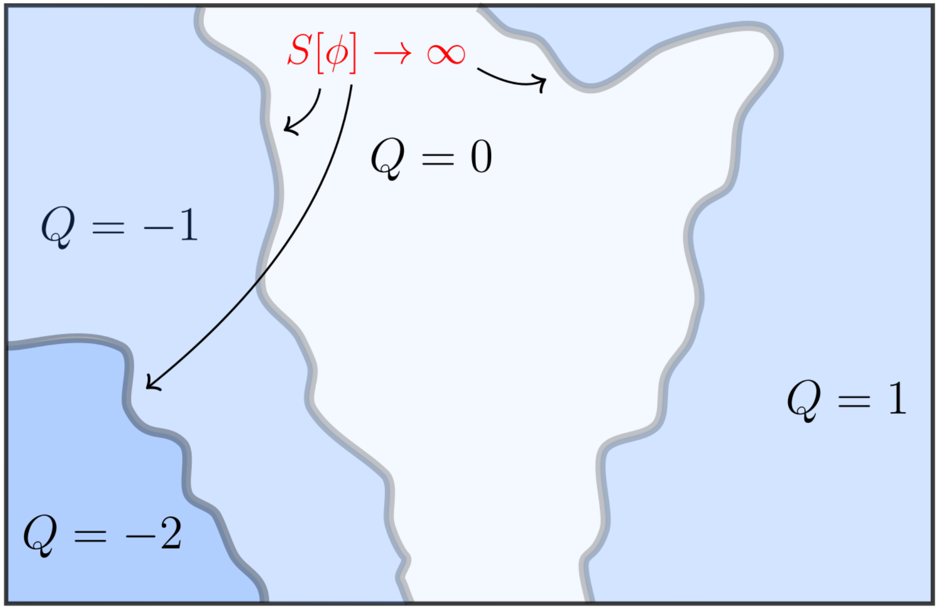
$N_f = 0$ results: fixed topology

But does HMC sample correctly observables at fixed topological sectors?



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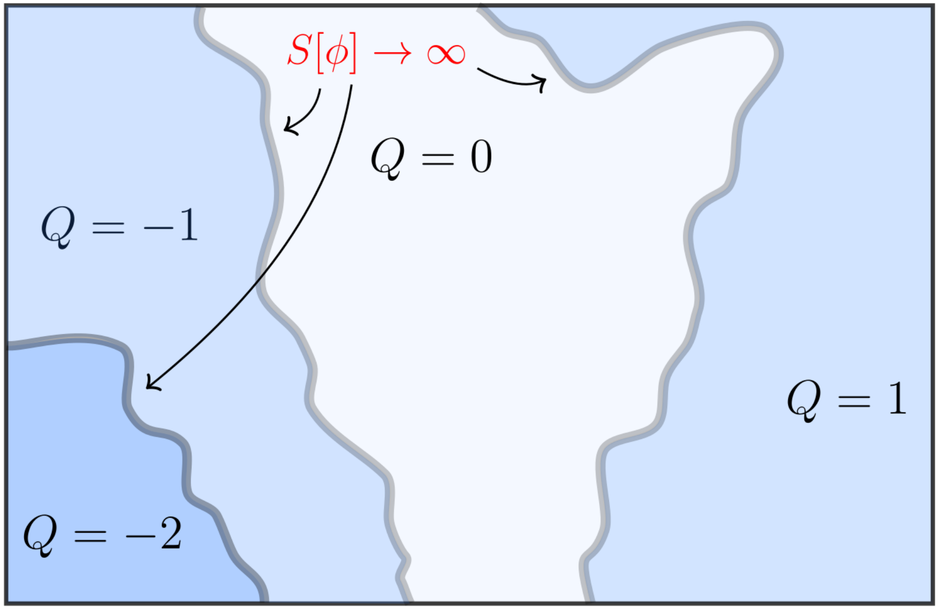

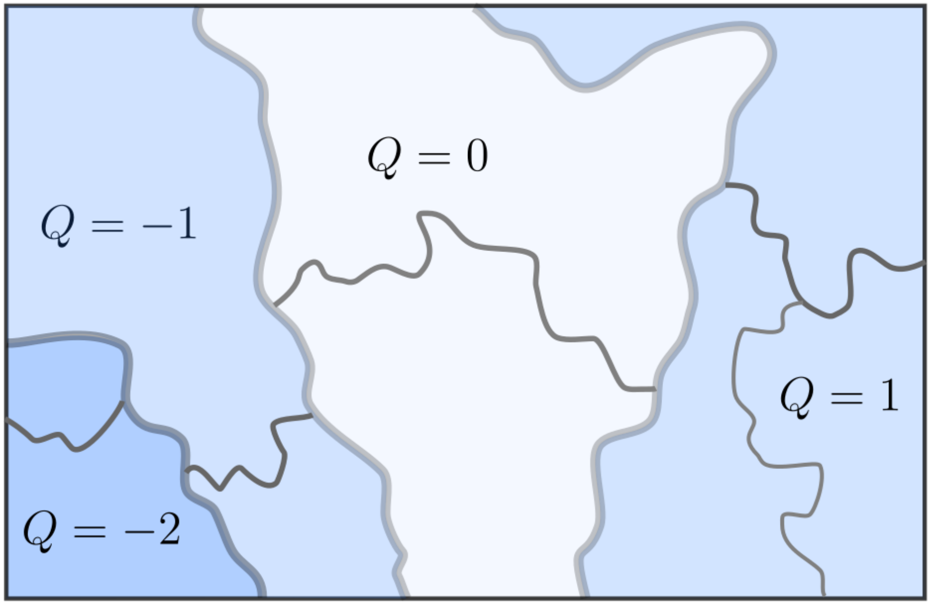

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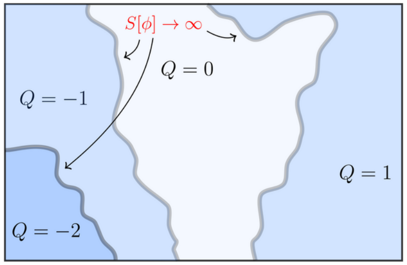

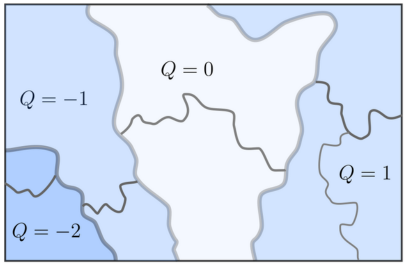

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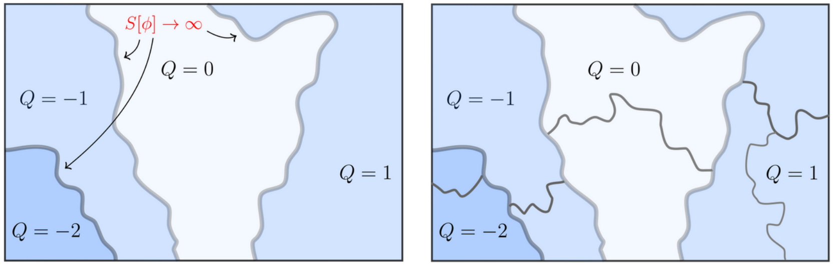

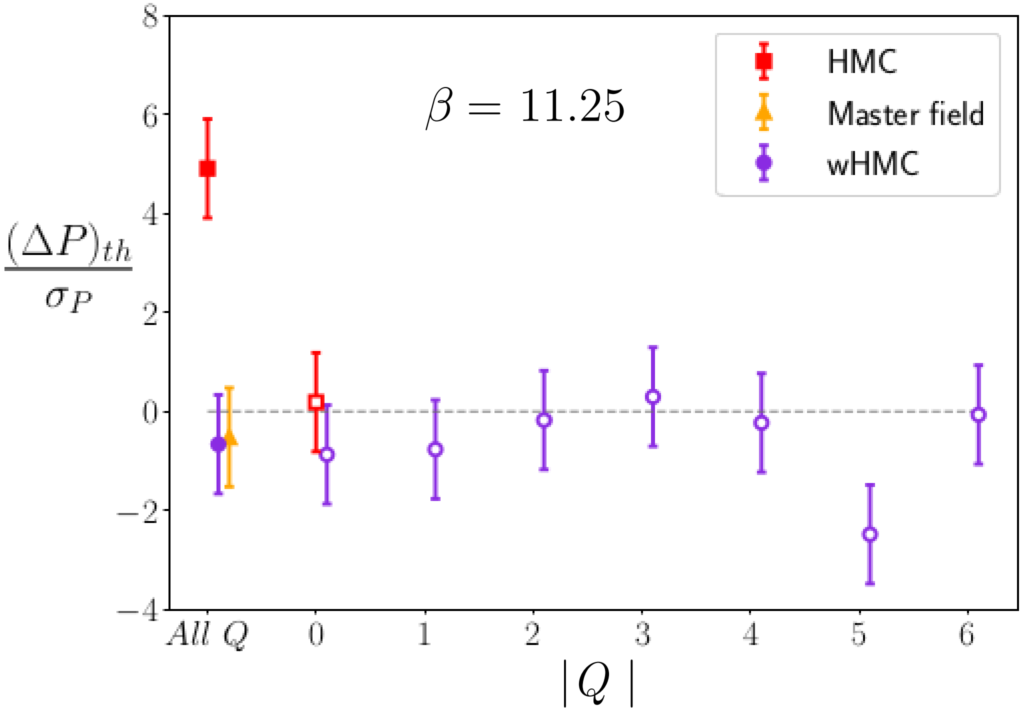

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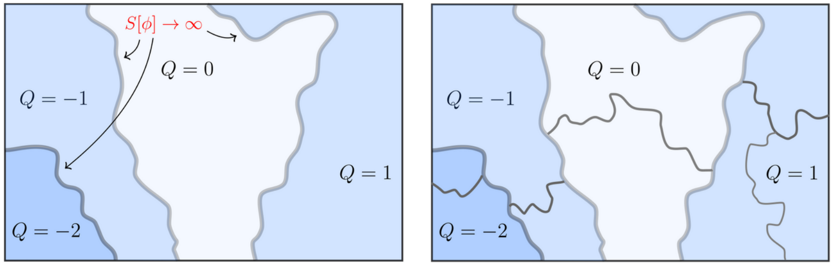

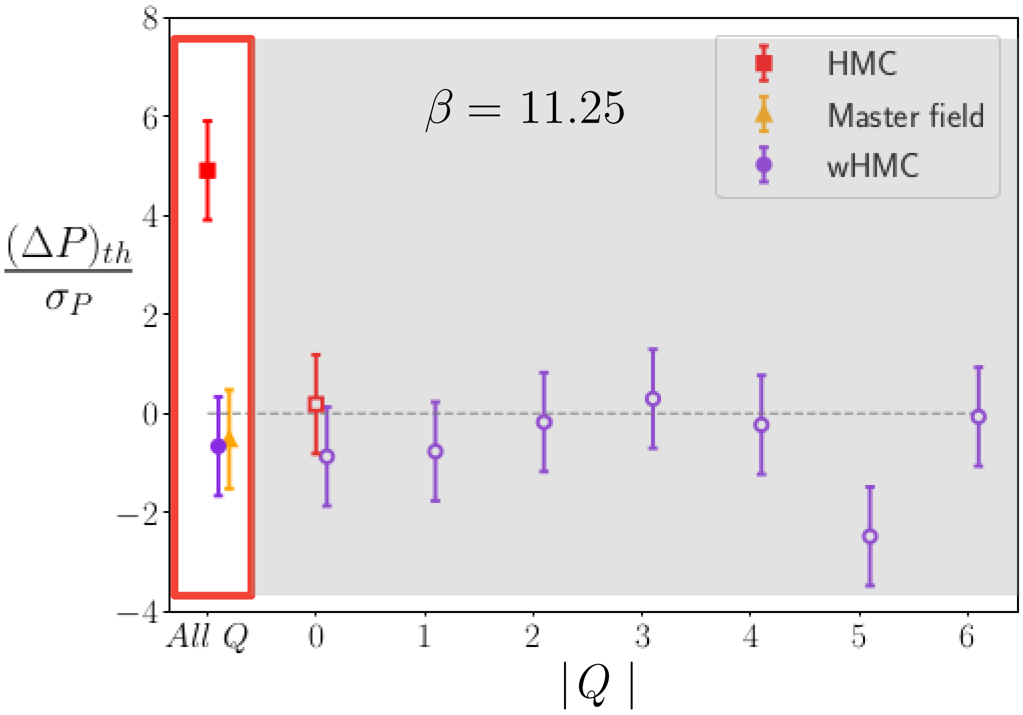

HMC gets wrong the final value of the plaquette

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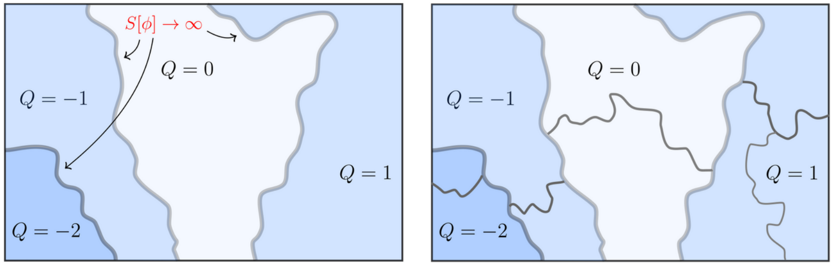

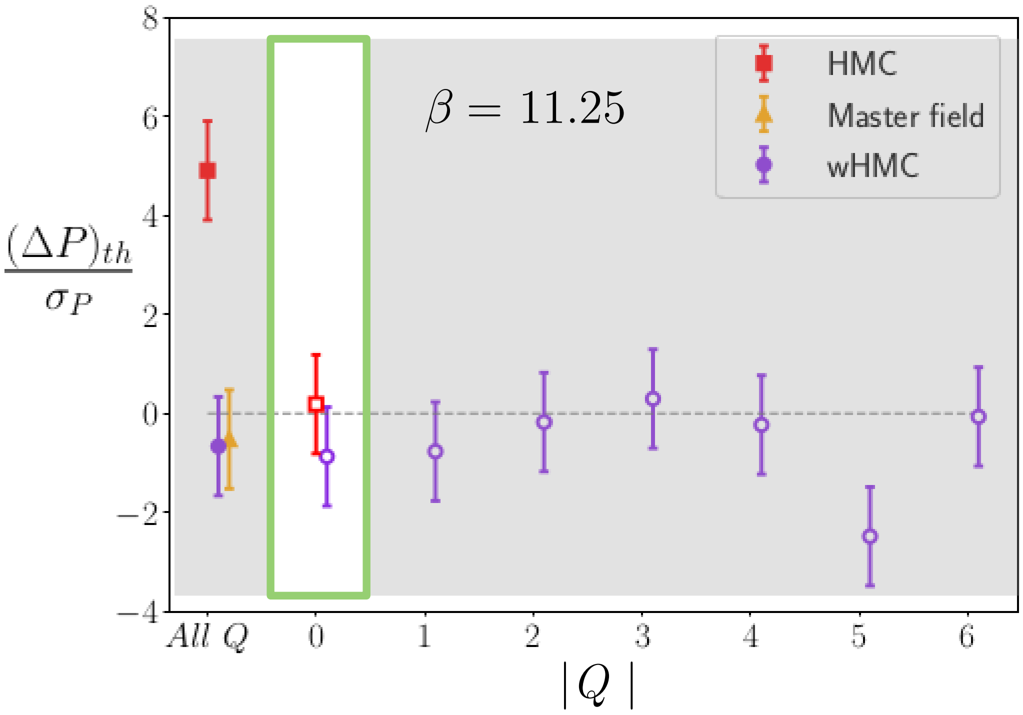

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but samples correctly the sector $Q = 0$

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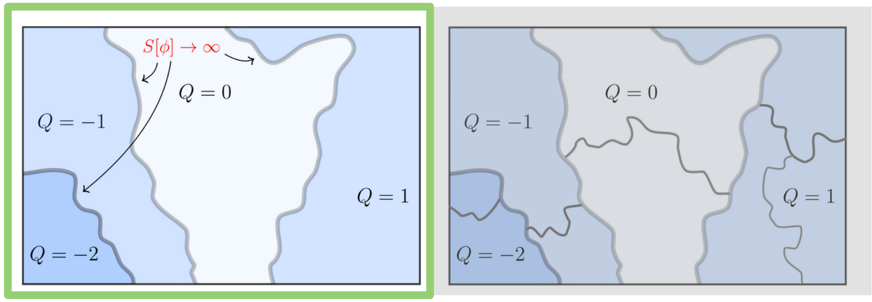
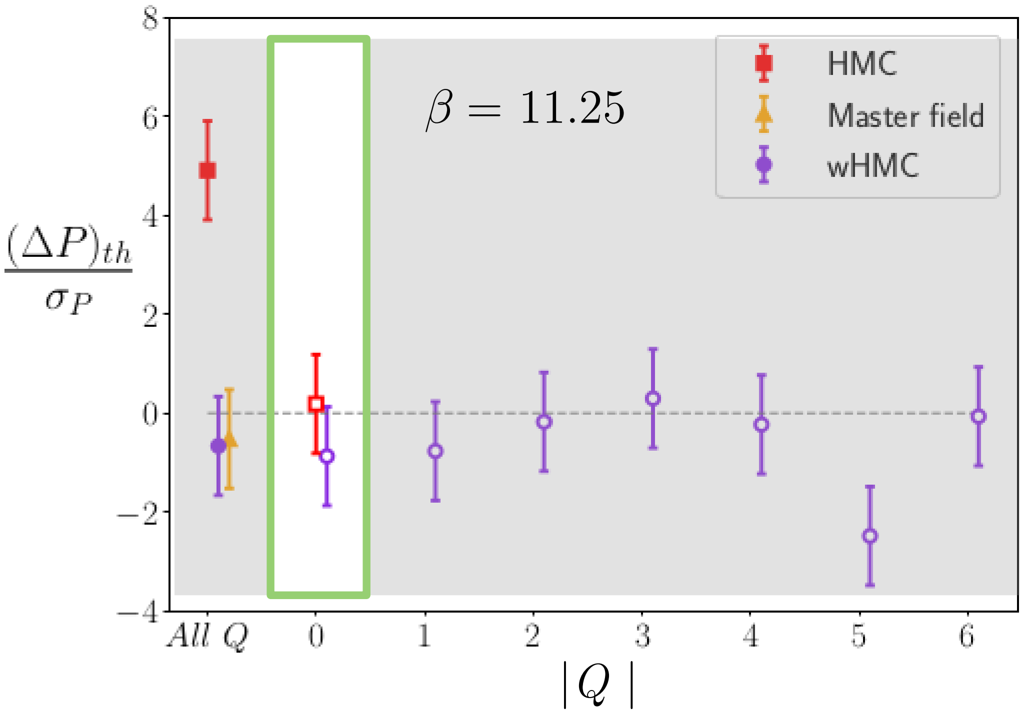


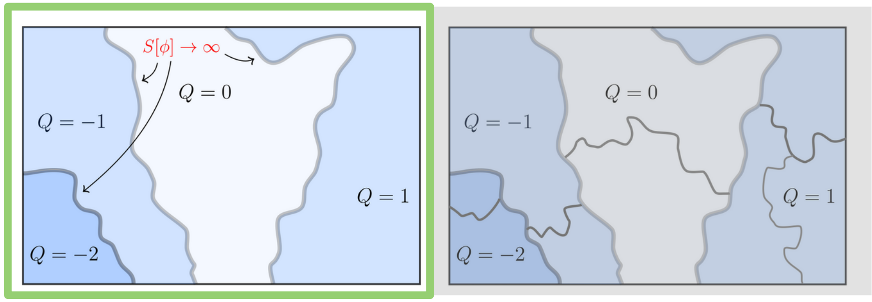


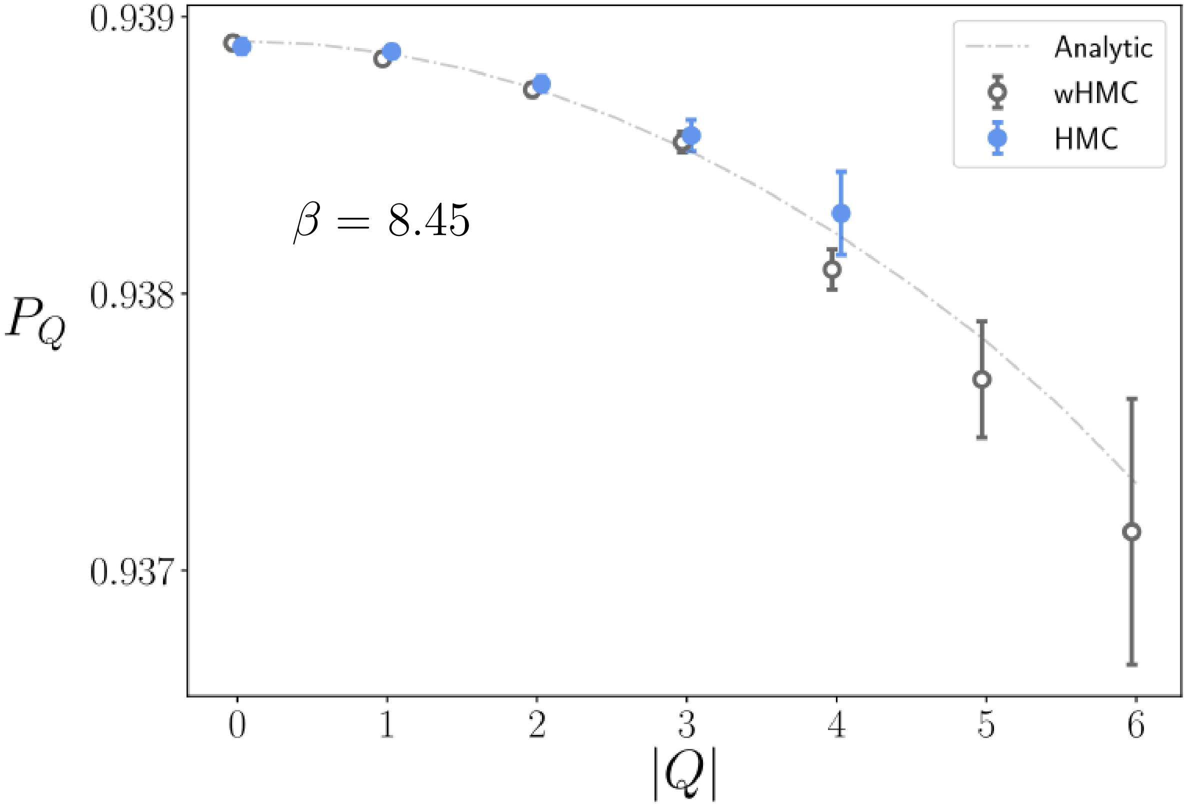
HMC gets wrong the final value of the plaquette

but samples correctly the sector $Q = 0$

$N_f = 0$ results: fixed topology

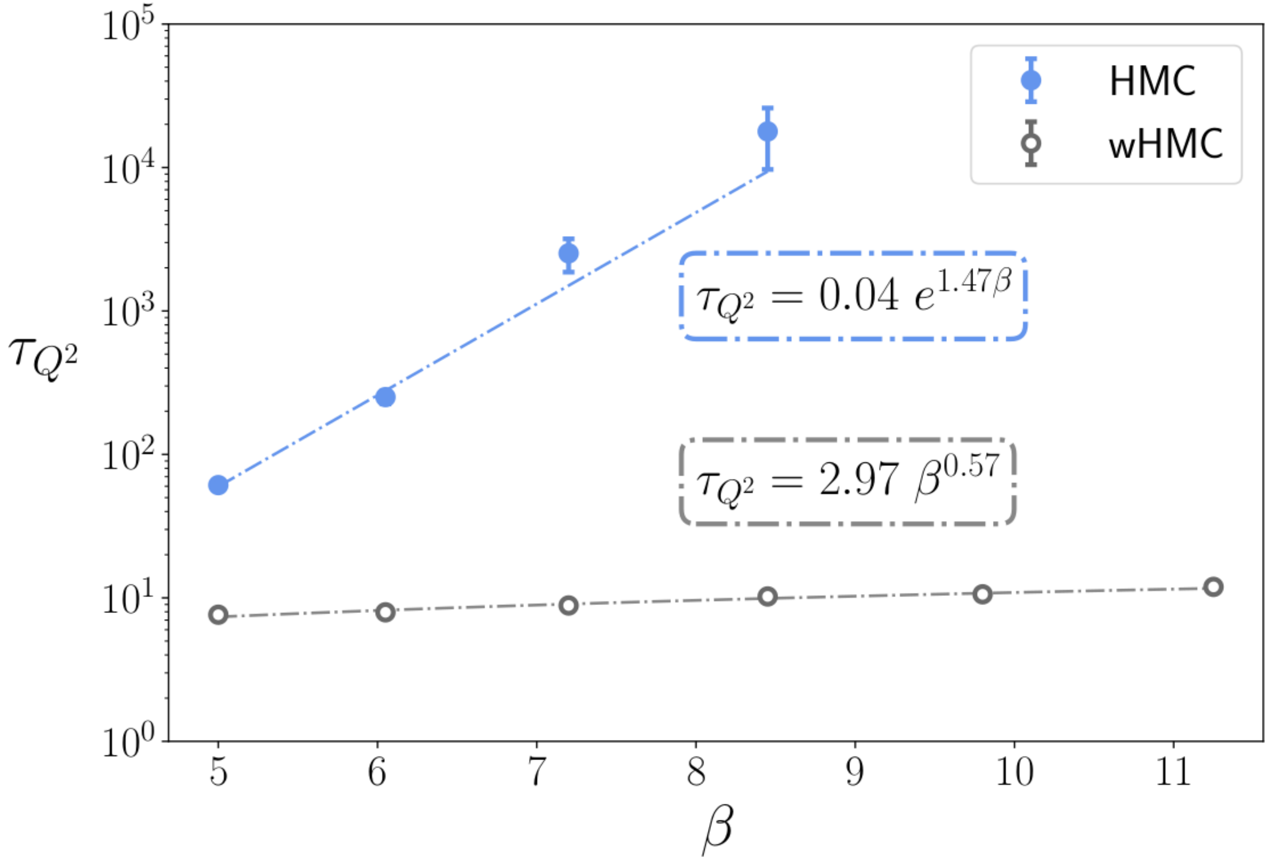
But does HMC sample correctly observables at fixed topological sectors?



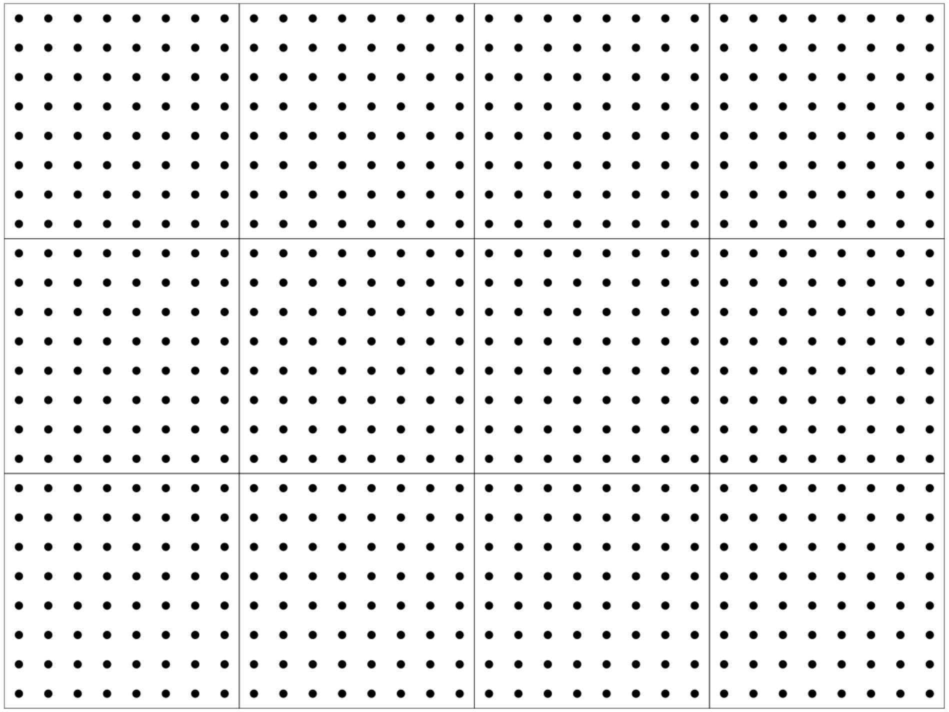


HMC samples correctly within each topological sector

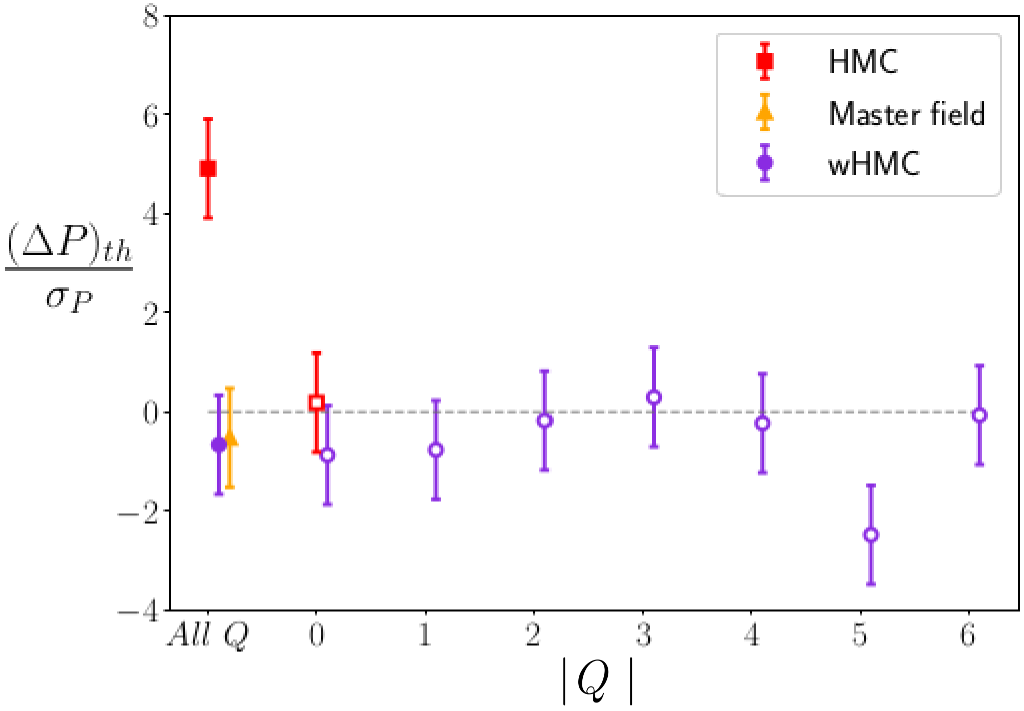
$N_f = 0$ results: scaling with a



- HMC autocorrelation increases exponentially
- wHMC increases only polynomially



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

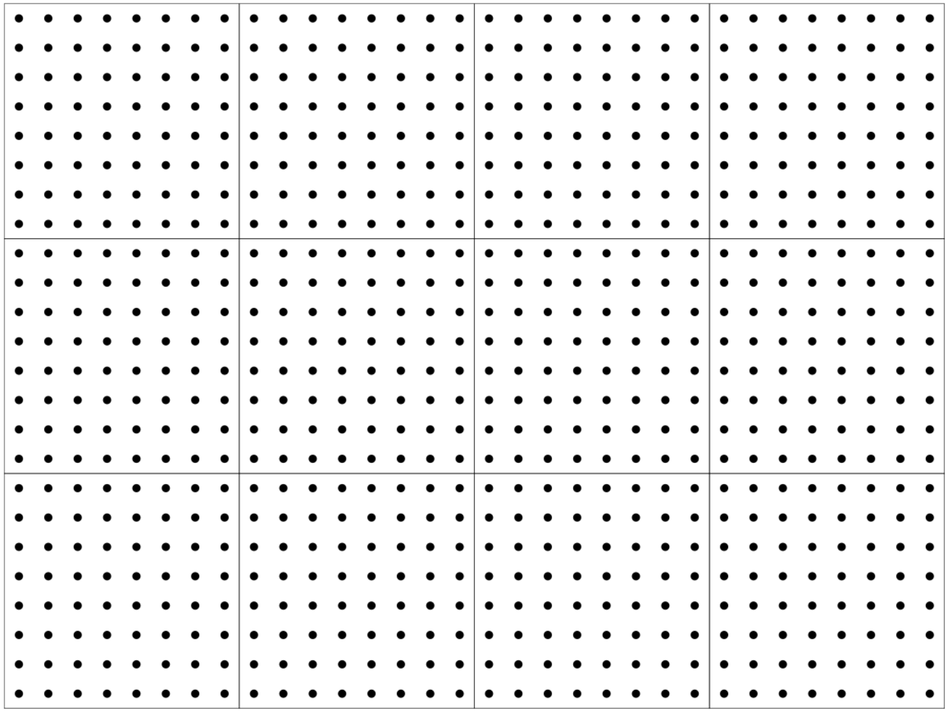


- Perform spacetime averages in huge lattices instead of Monte-Carlo-time averages

$$\langle\langle \mathcal{O}(x) \rangle\rangle = \frac{1}{V}\sum_z \mathcal{O}(x+z) \qquad \langle\langle \mathcal{O}(x) \rangle\rangle = \langle \mathcal{O}(x) \rangle + \mathrm{O}(V^{-1/2})$$

- Q is fixed, but does not suffer from topology freezing: $O(V^{-1})$ effects
- Can extract observables from one single configuration, but hard to thermalize!

Master fields



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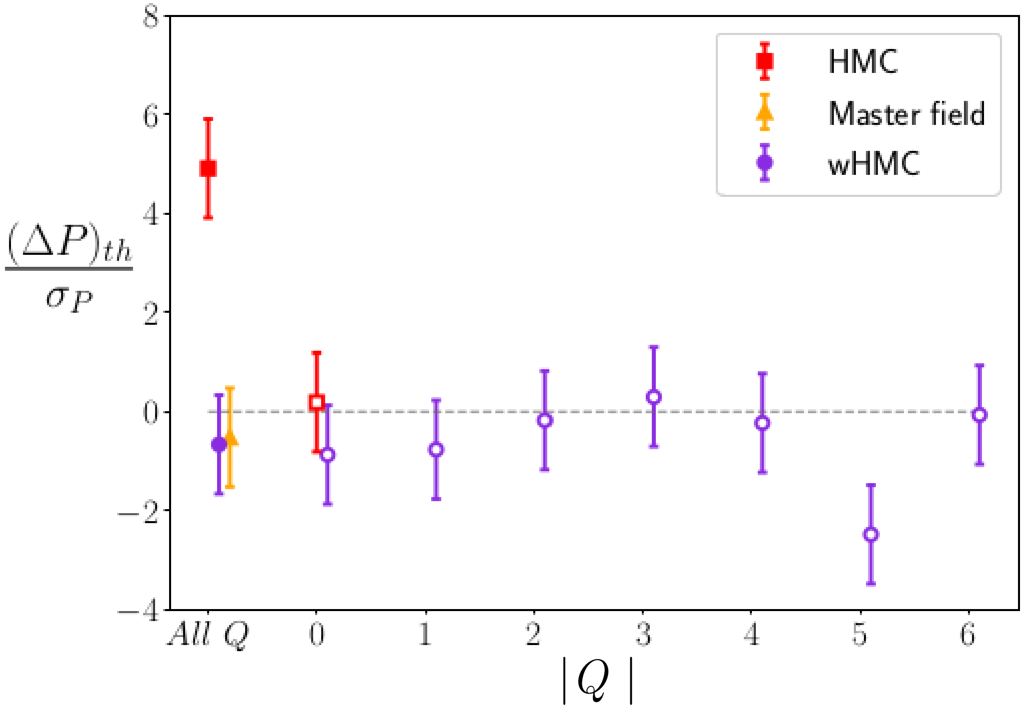
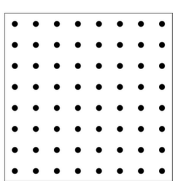
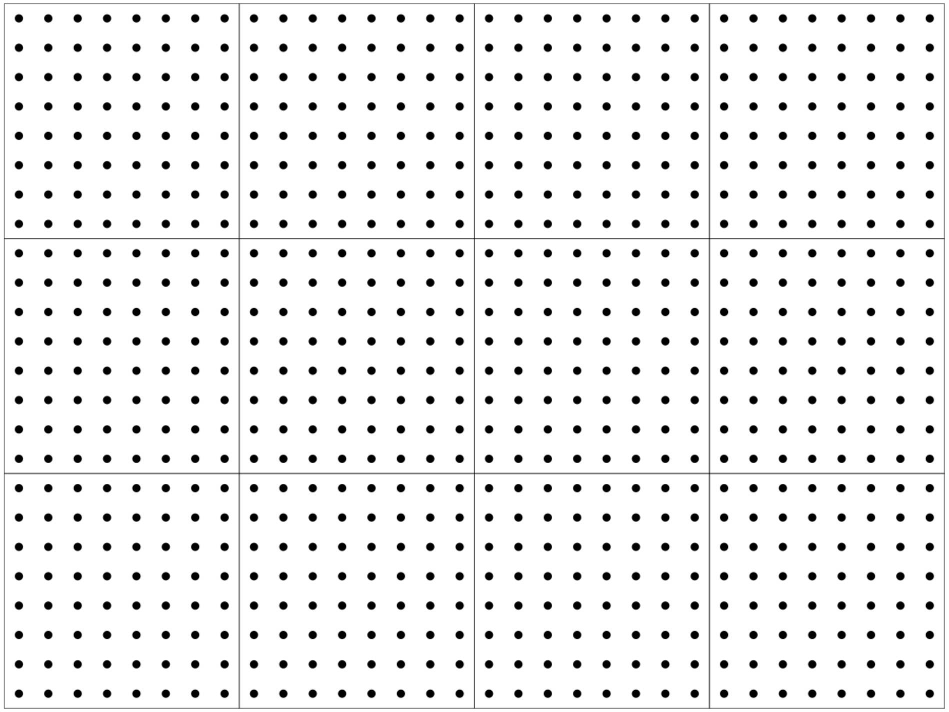


Thermalization procedure:



☆ Unfold with reflections



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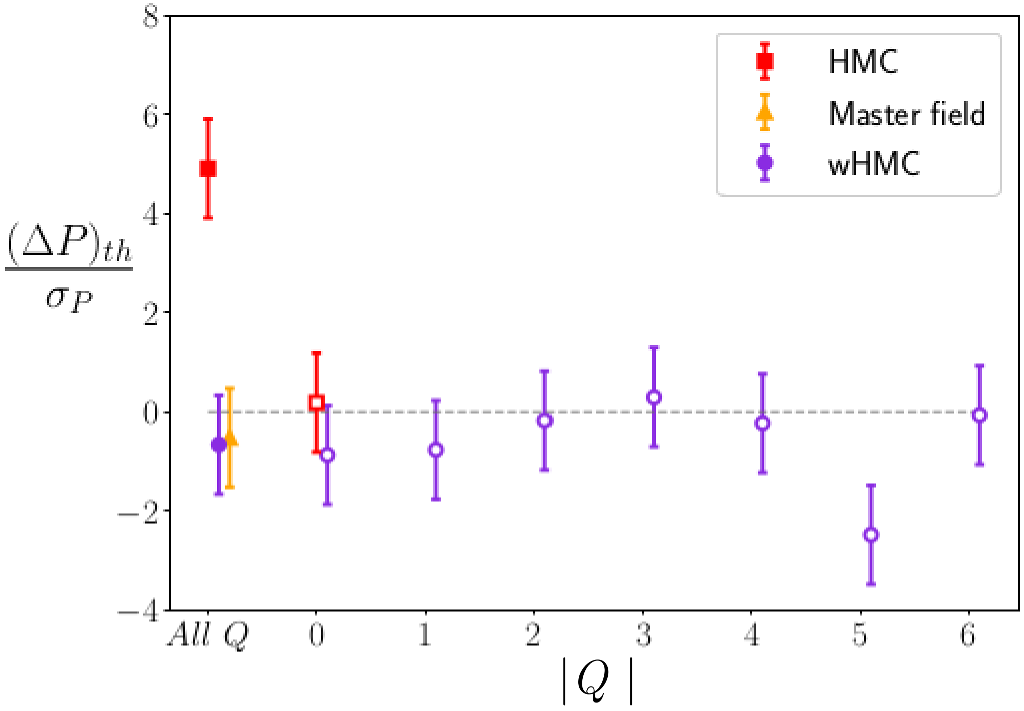

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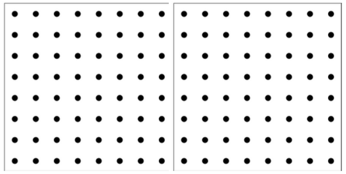

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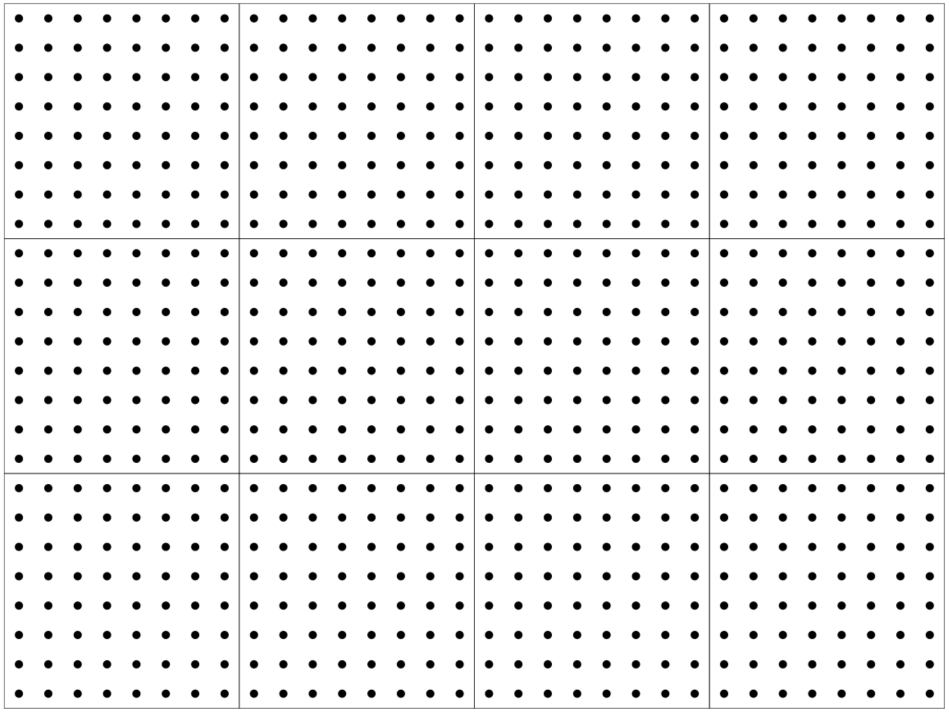

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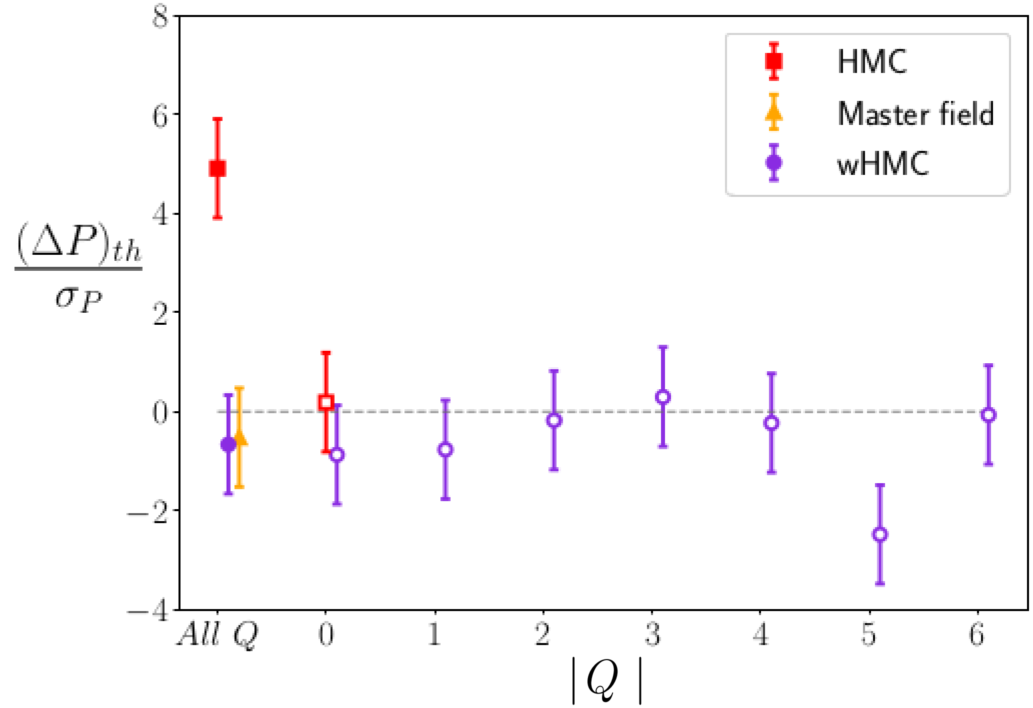

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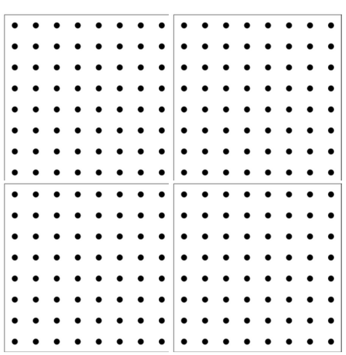
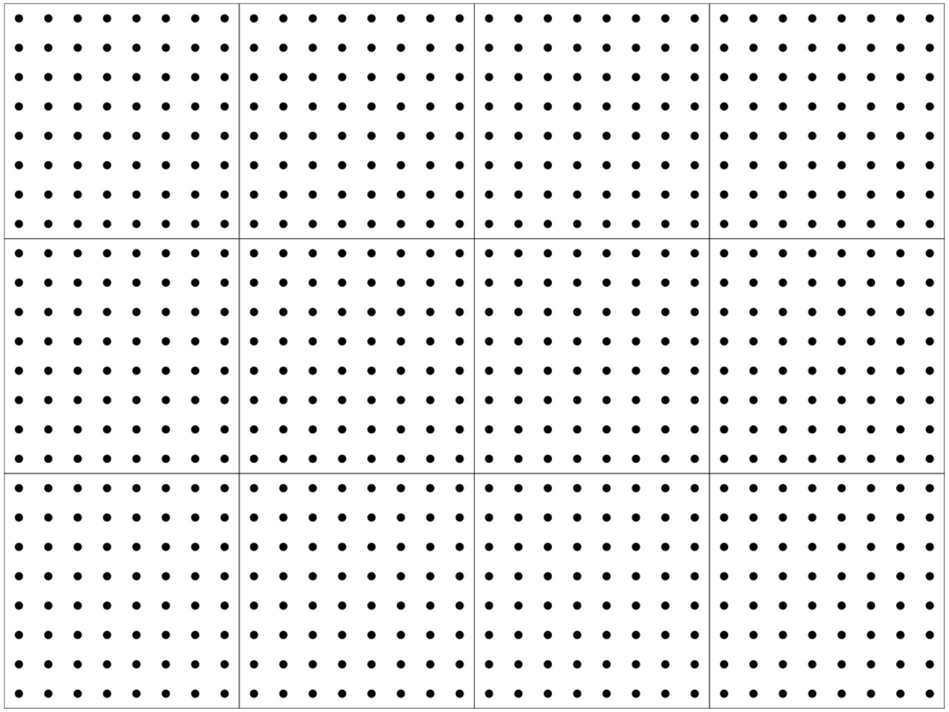
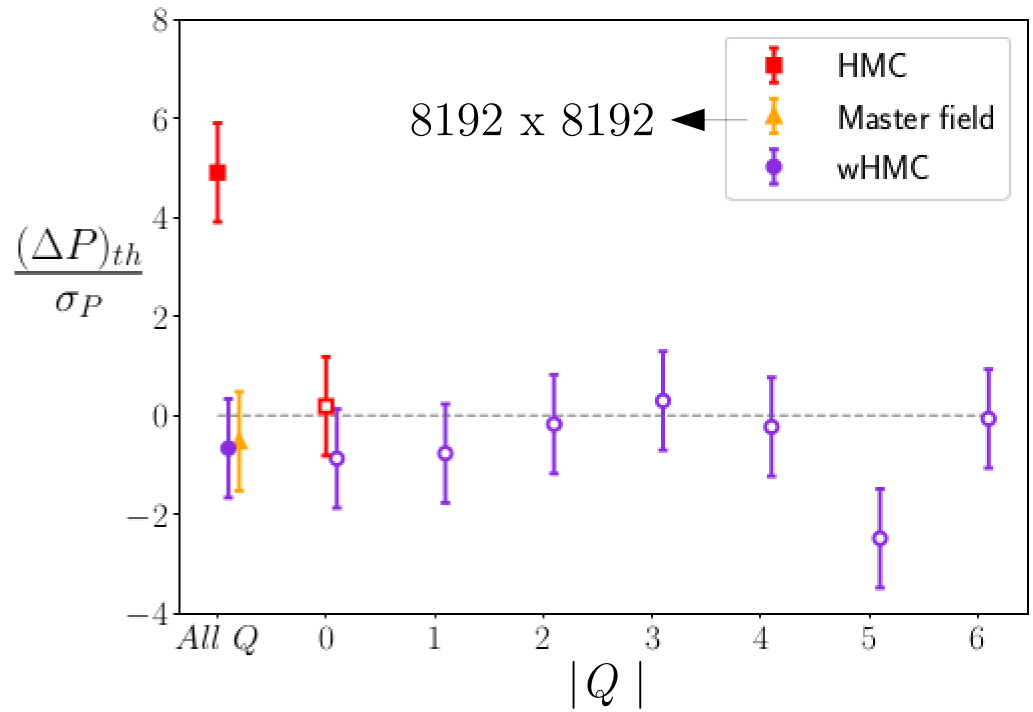


- Unfold with reflections
- This way low charge density is ensured with high probability
- Cost of the algorithm comes only from the thermalization

Master fields





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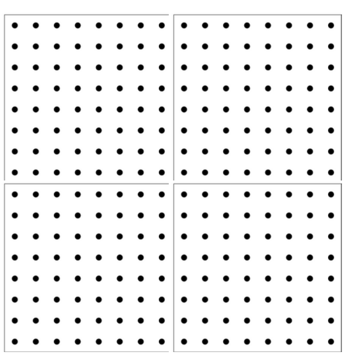

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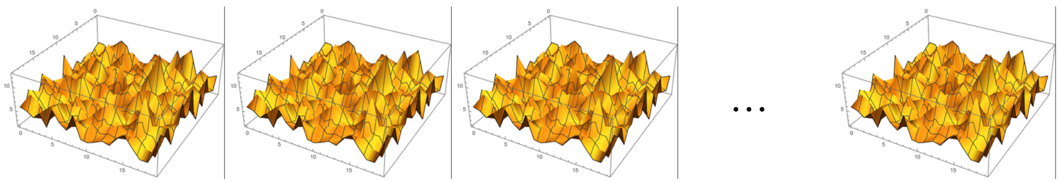
Master fields: computing the plaquette with Γ method

U. Wolff, Comput. Phys. Commun. 156, 143 (2004)

Review: Normal MC simulation



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$$U_1,\ U_2,\ U_3,\ \ldots,\ U_N$$

2. Compute plaquette P on each of them

$$P_1,\ P_2,\ P_3,\ \ldots,\ P_N$$

Central value: $$\overline{P} = \frac{1}{N}\sum_{i}^{N} P_i$$

(average over MC time)

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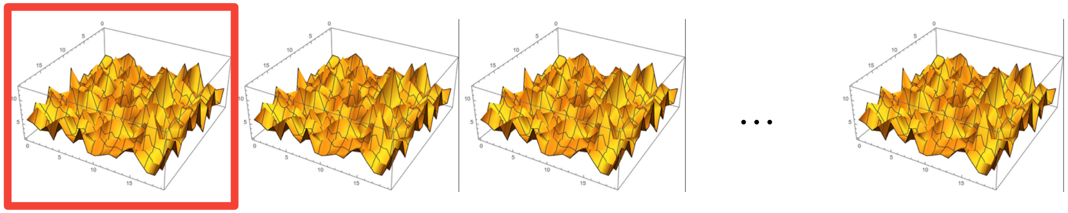

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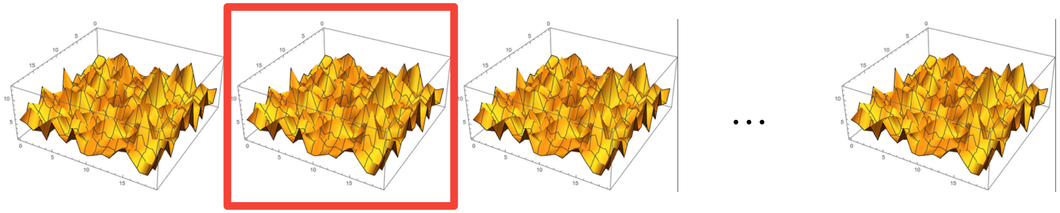

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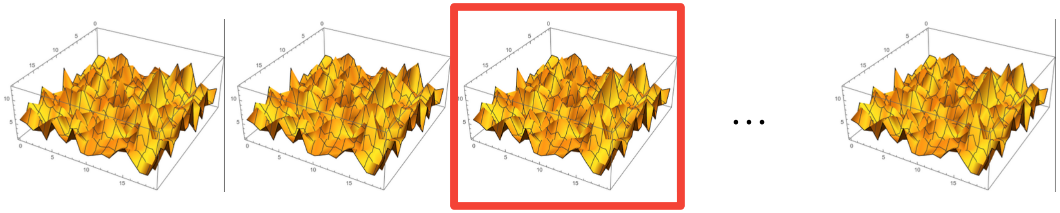

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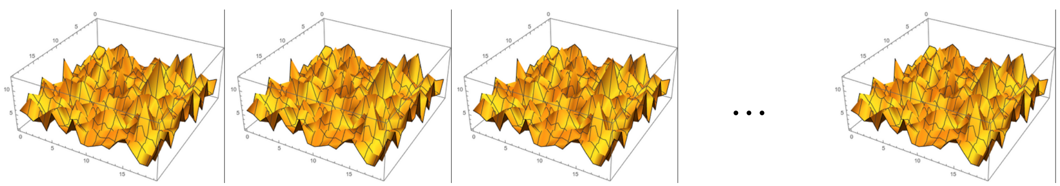

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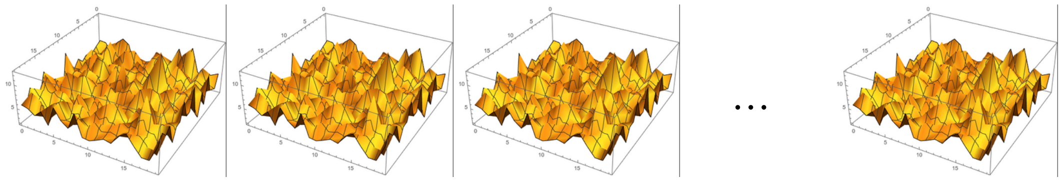

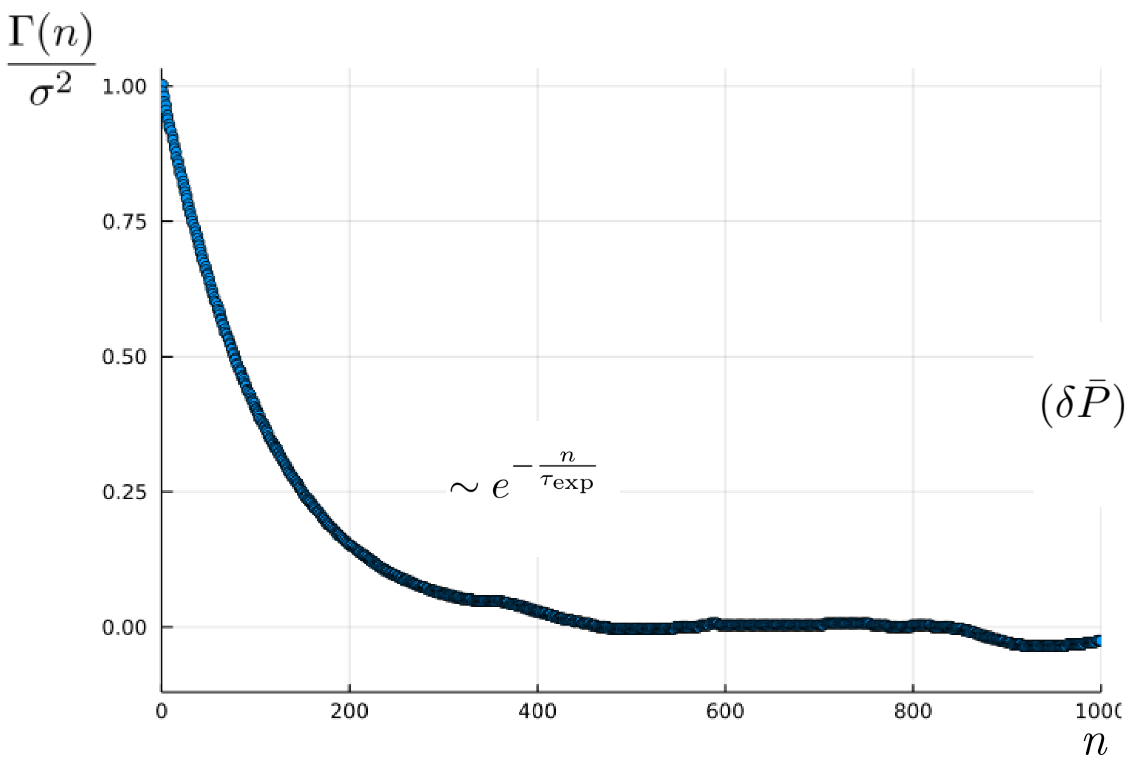

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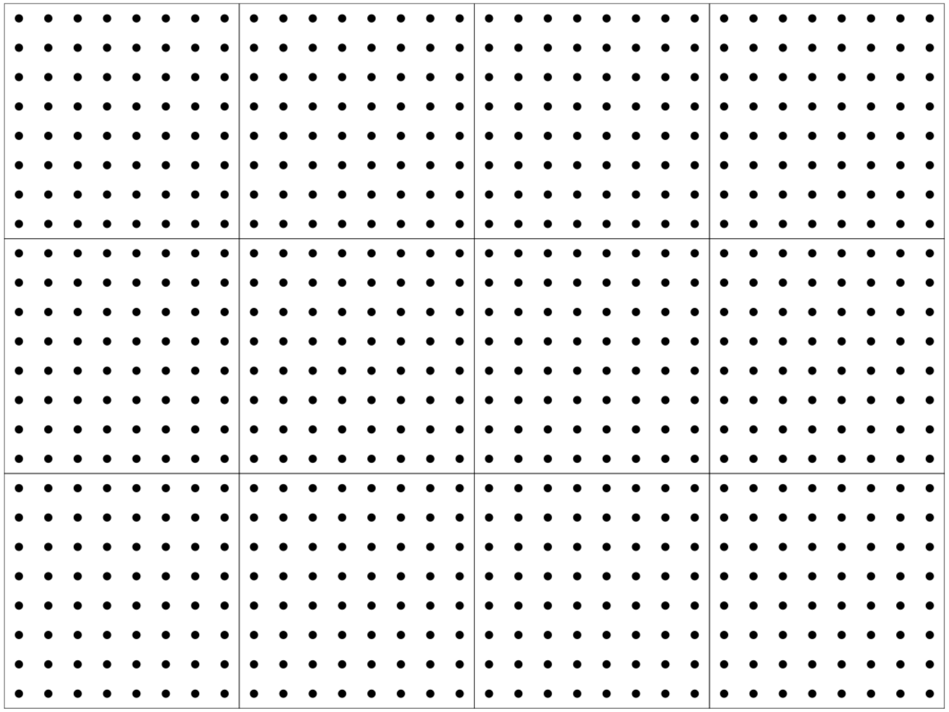

Master field simulation

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   $P(0,0)$, $P(0,1)$, $P(0,2)$, ...

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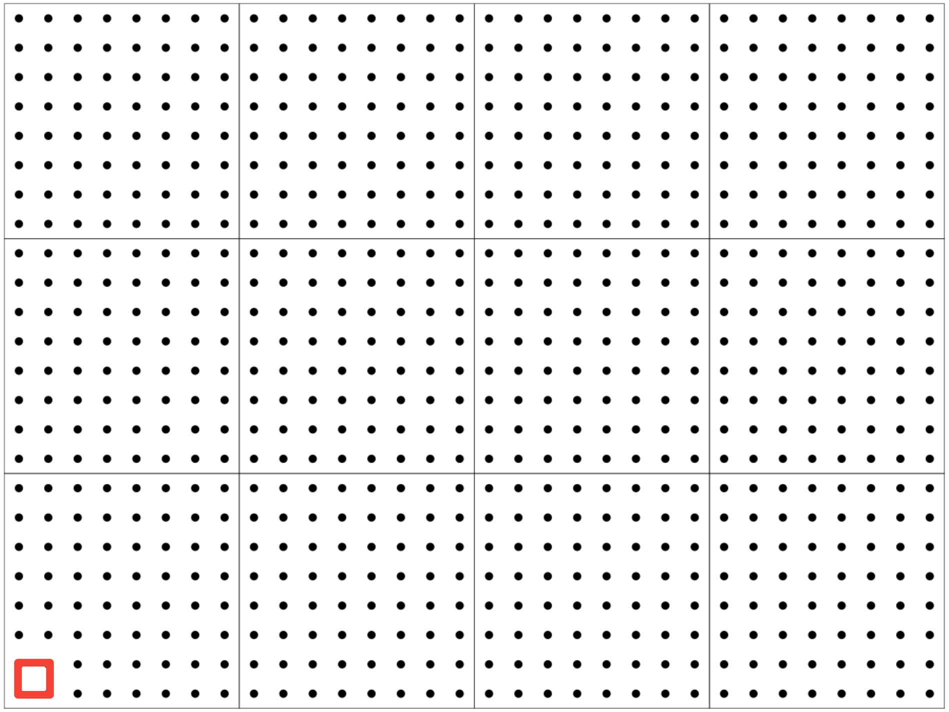

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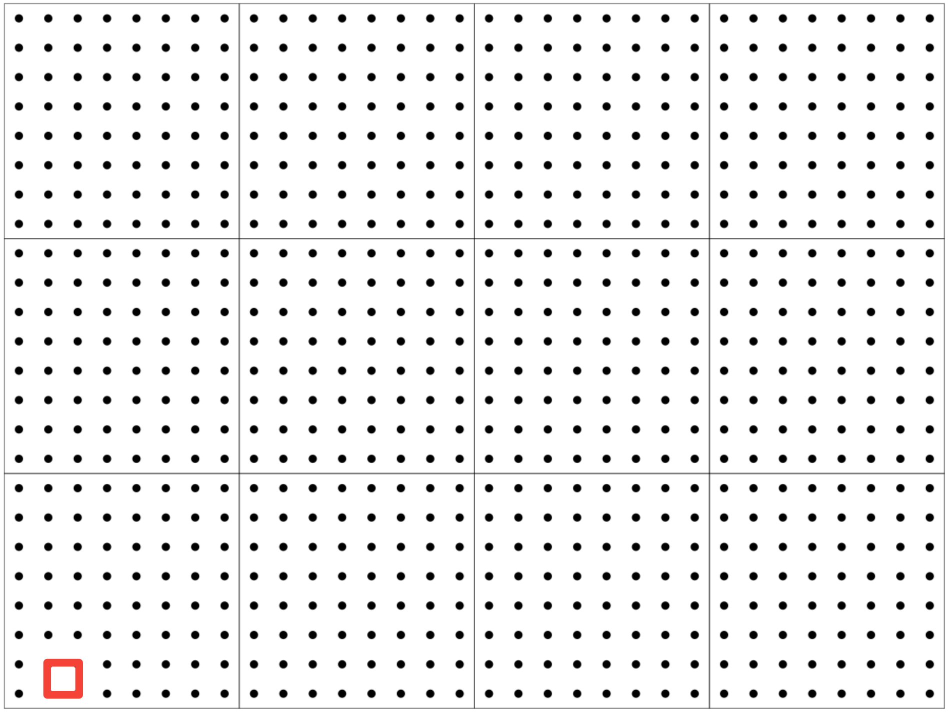

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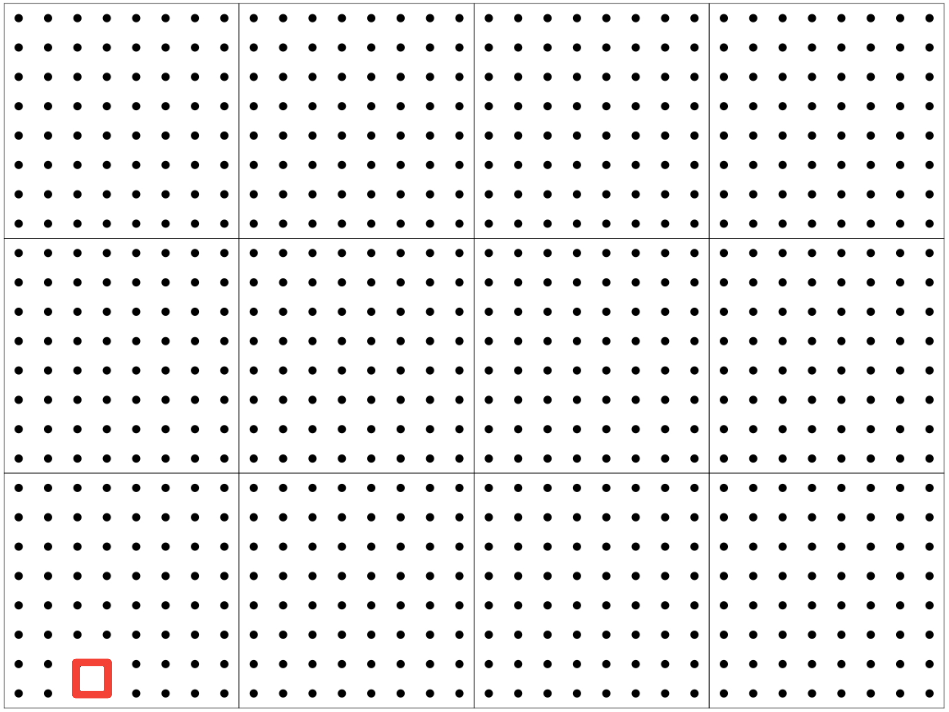

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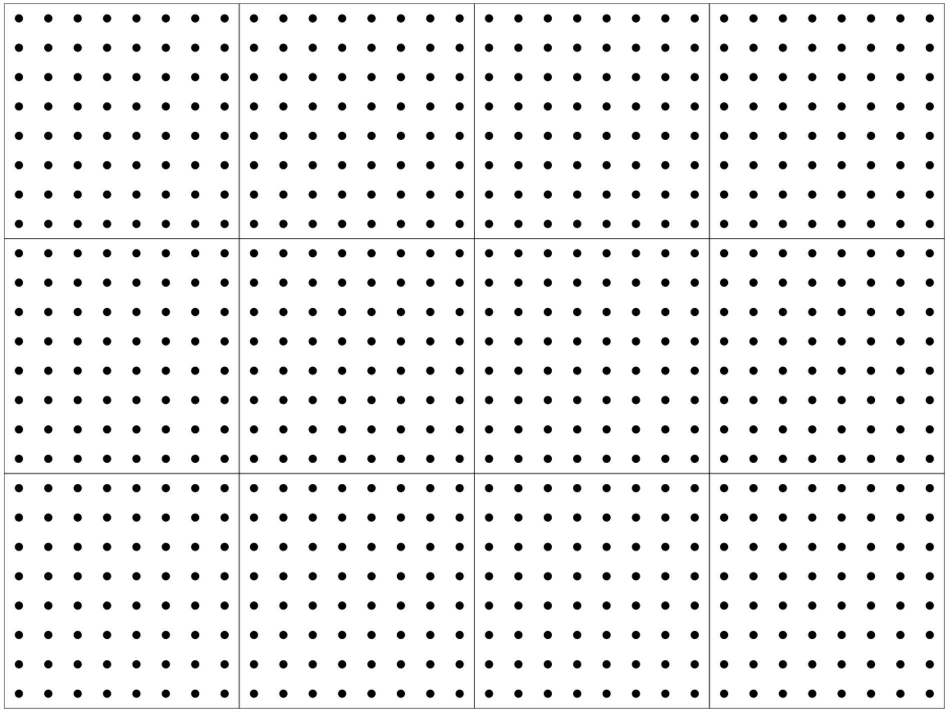

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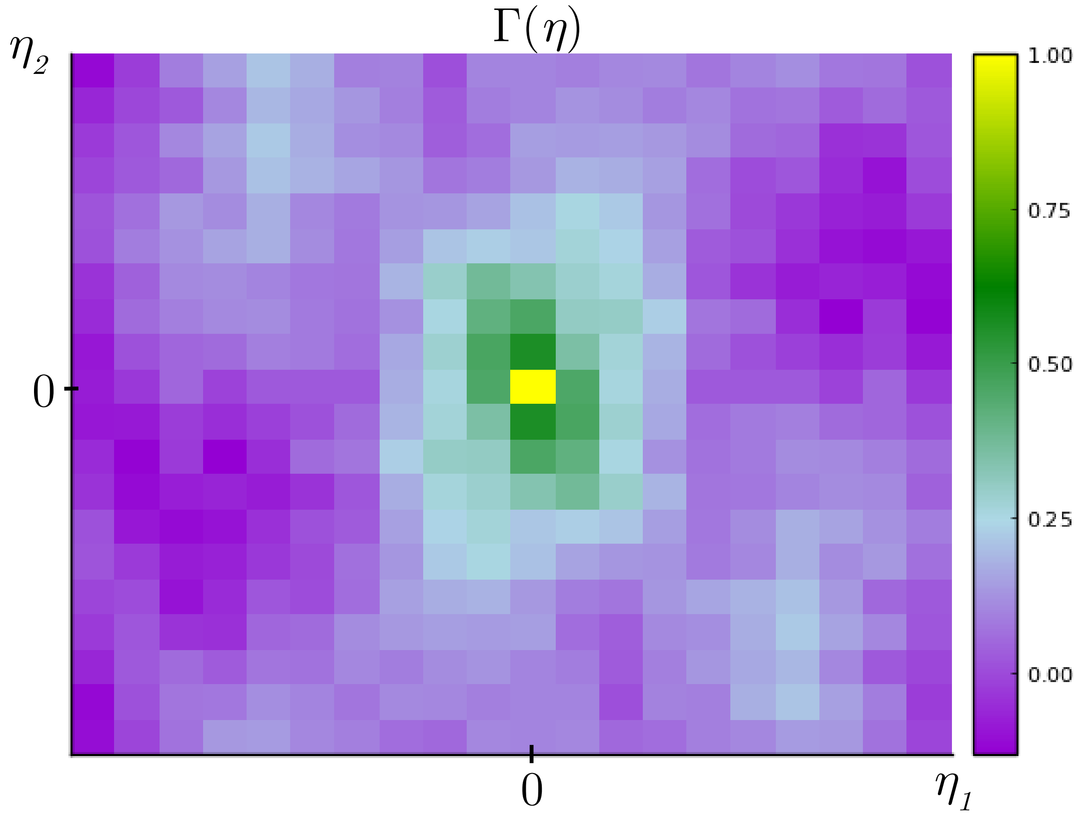

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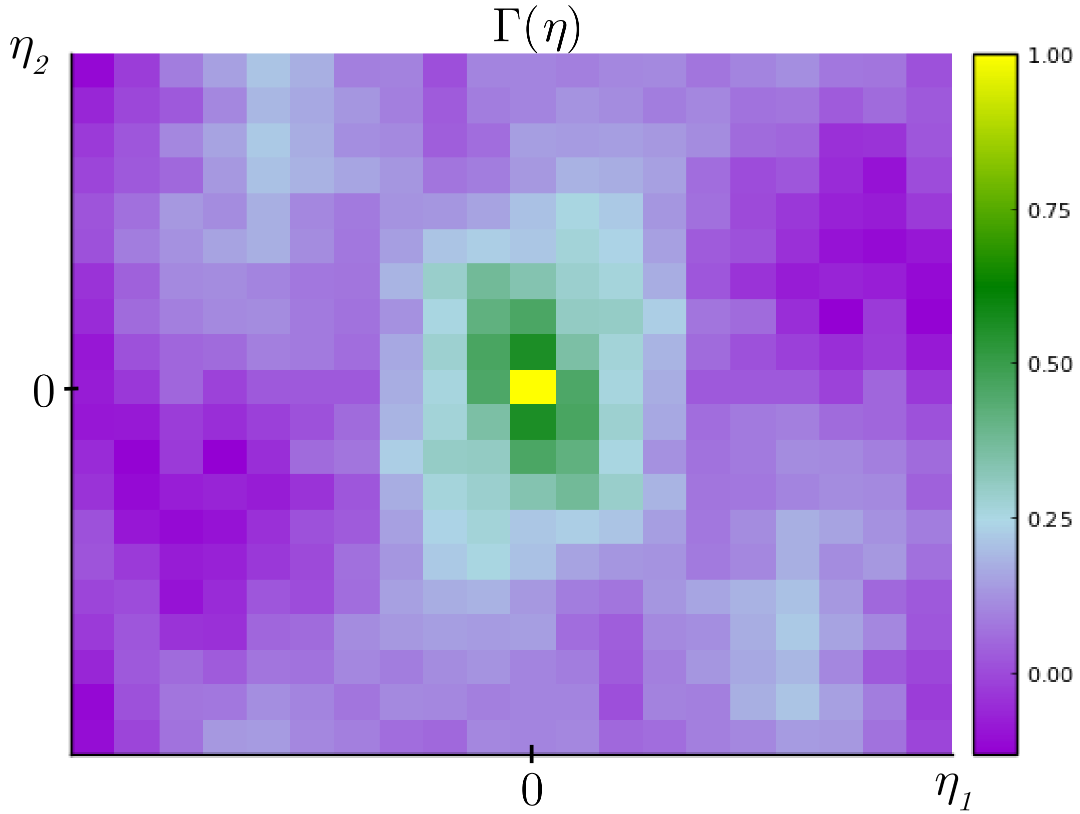

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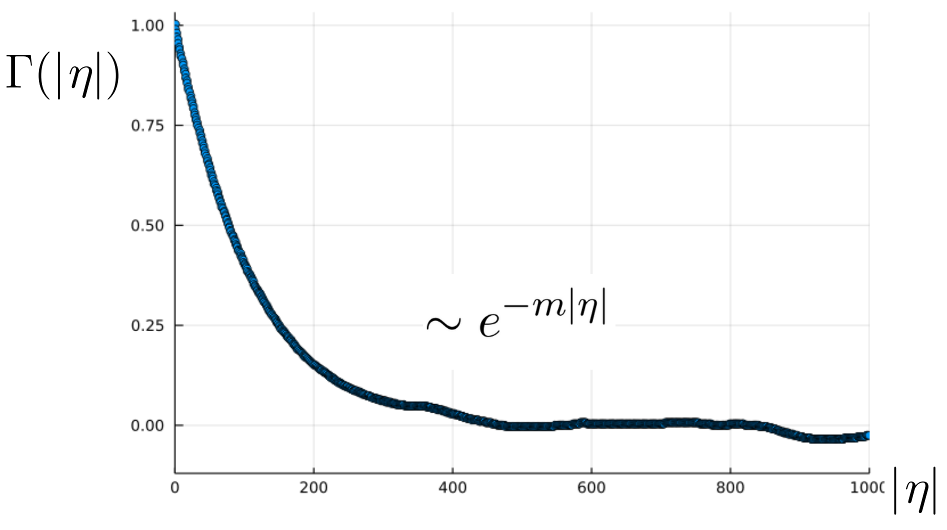

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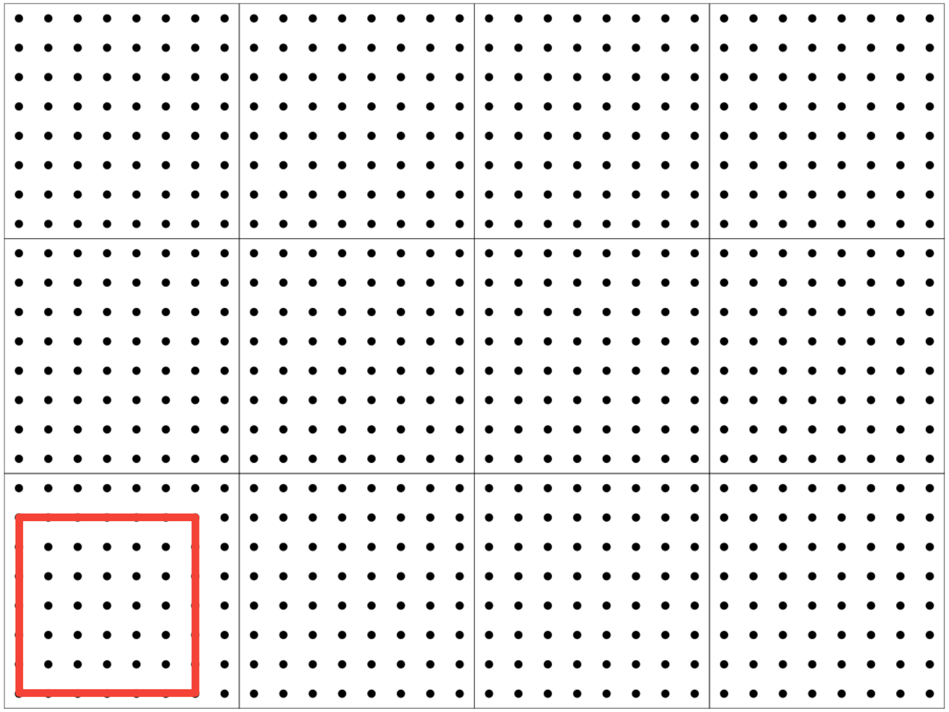
Master fields: computing non-local observable



MC simulation | **Master field simulation**

☆ Topological susceptibility:

$$\chi_t = \sum_y \langle q(y)q(0)\rangle$$

sum over whole lattice

$$\chi_R(x) = \sum_{|y_i|<R} q(x)q(x+y)$$

truncate sum up to $R > \xi$

☆ Uncertainty: $$(\delta\bar{\chi})^2 = \frac{1}{V}\sum_{\eta=0}\frac{1}{V}\sum_x\left[\sum_{|z_{1,i}|<R} q(x)q(x+z_1)-\bar{\chi}\right]\left[\sum_{|z_{2,i}|<R} q(x+\eta)q(x+\eta+z_2)-\bar{\chi}\right]$$

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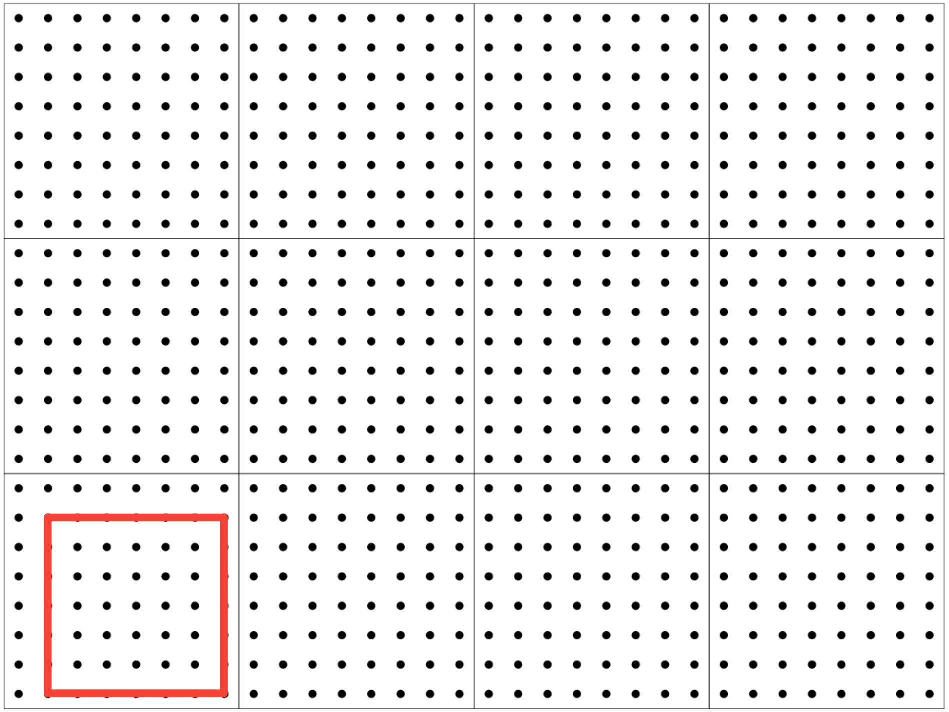

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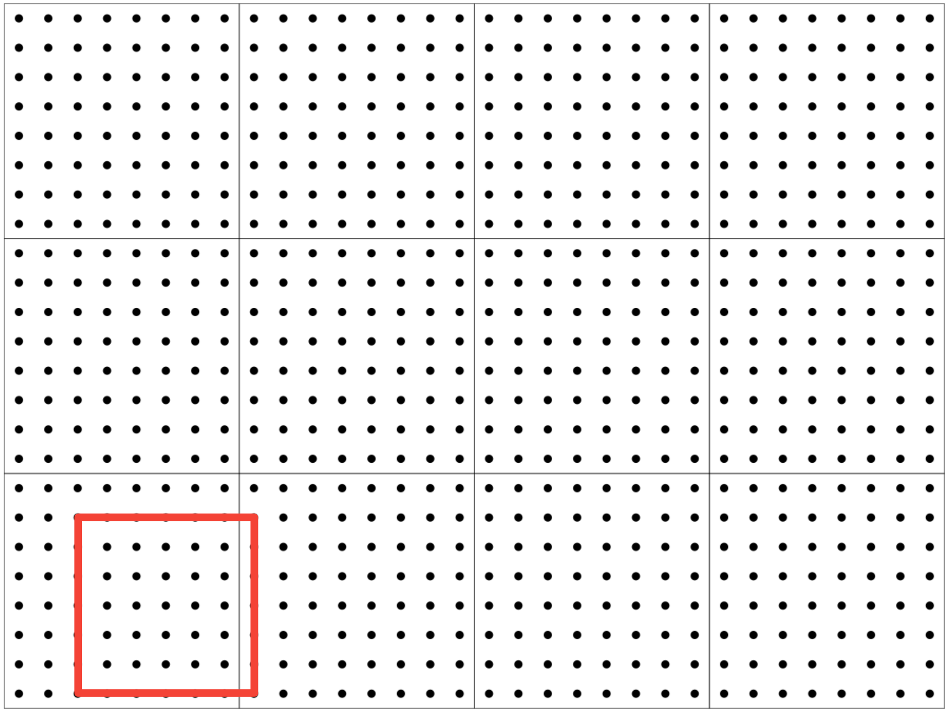

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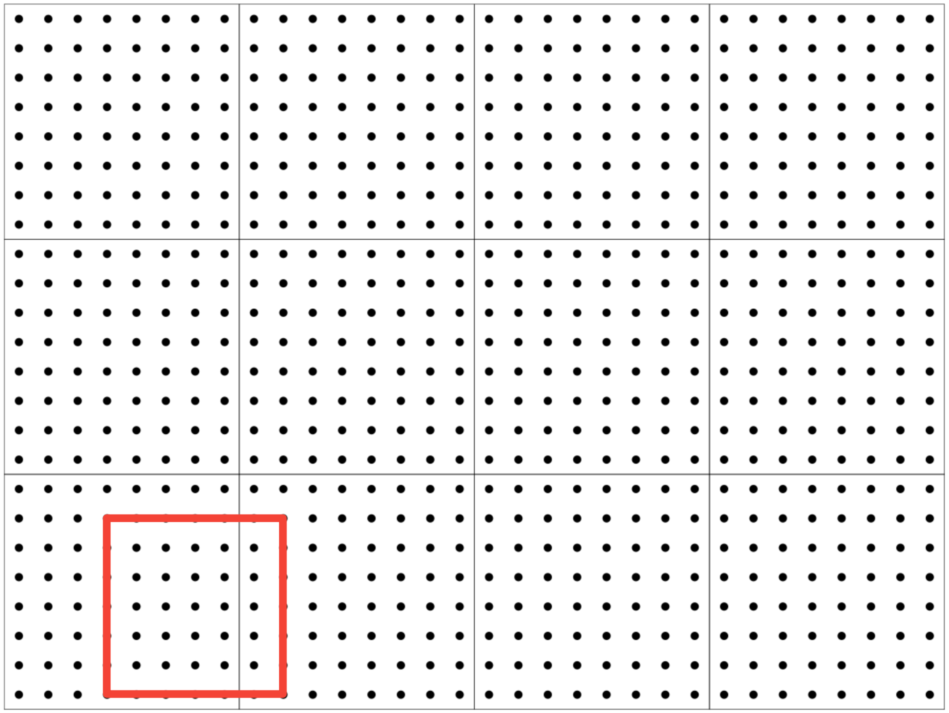

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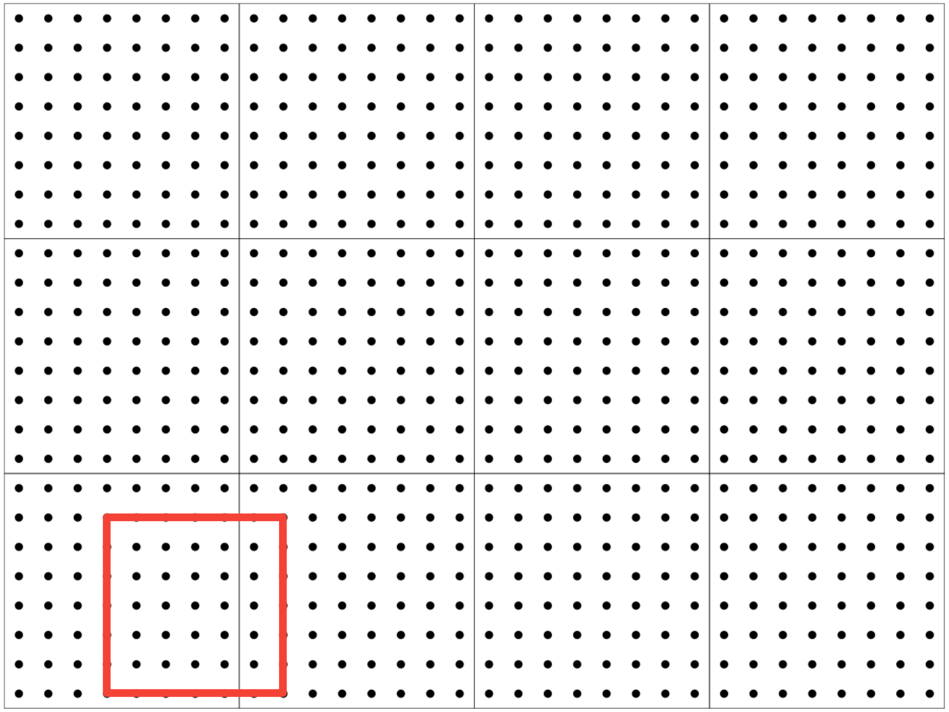

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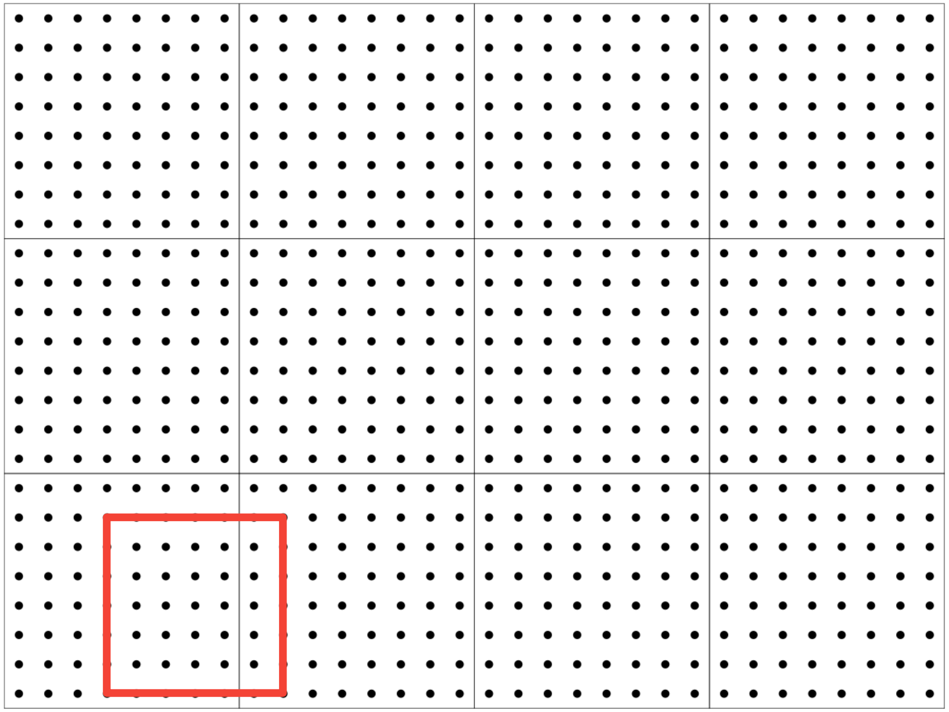
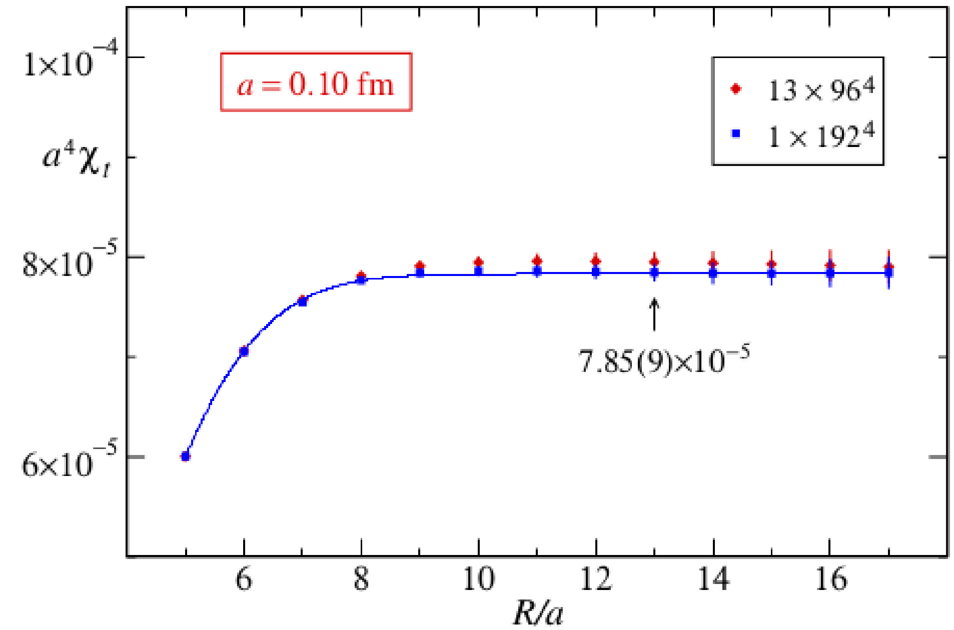
☆ Statistical error increases with R

☆ $\chi_t = \langle\langle \chi_R \rangle\rangle + \delta(R) + O(V^{-1/2})$

Master fields: computing non-local observable



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

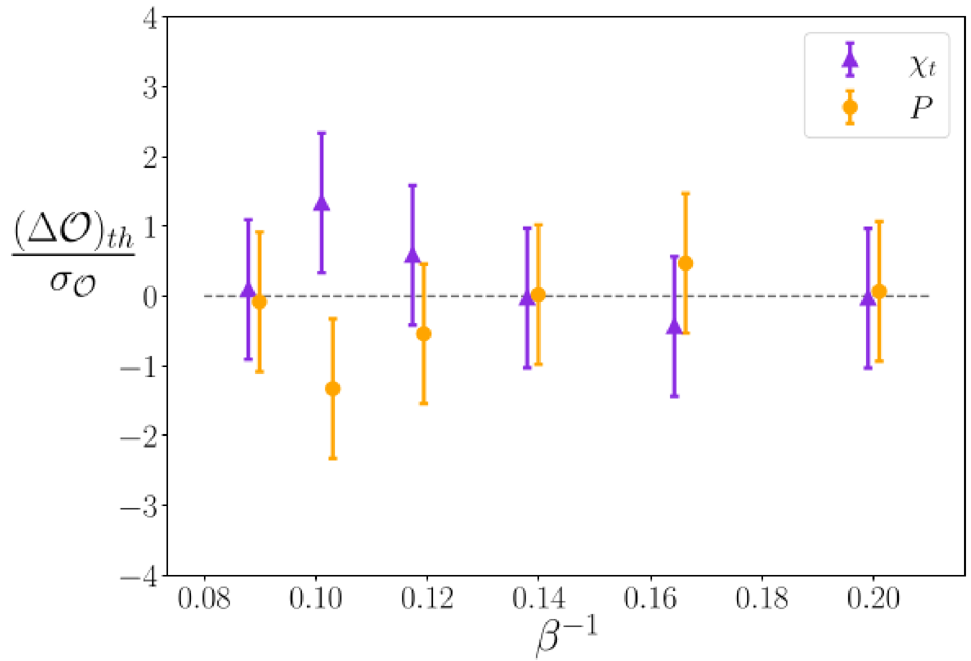


	MC simulation	**Master field simulation**
☆ Topological susceptibility:	$\chi_t = \sum_y \langle q(y)q(0)\rangle$ sum over whole lattice	$\chi_R(x) = \sum_{\lvert y_i\rvert<R} q(x)q(x+y)$ truncate sum up to $R > \xi$

☆ Statistical error increases with R

☆ $\chi_t = \langle\langle \chi_R \rangle\rangle + \delta(R) + O(V^{-1/2})$

Master fields: U(1) in 2D

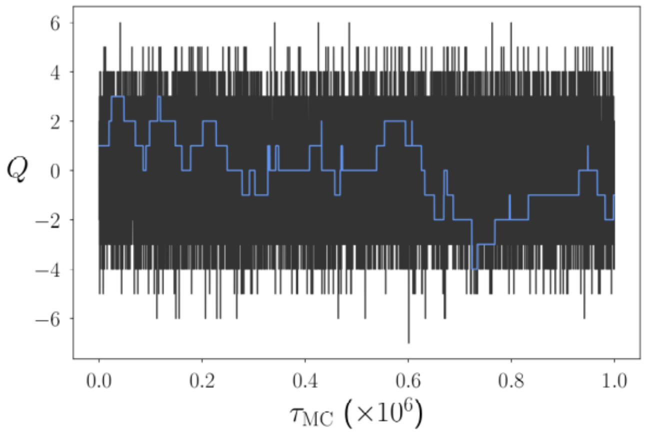


$$\chi_R(x) = \sum_{|y_i|<R} q(x)q(x+y) \qquad \frac{\mathrm{Var}[\chi_R(x)]}{\mathrm{Var}[\chi_0(x)]} \approx 1 + 2R^2$$

- In pure gauge U(1) there is no correlation length ⇒ choose $R = 0$

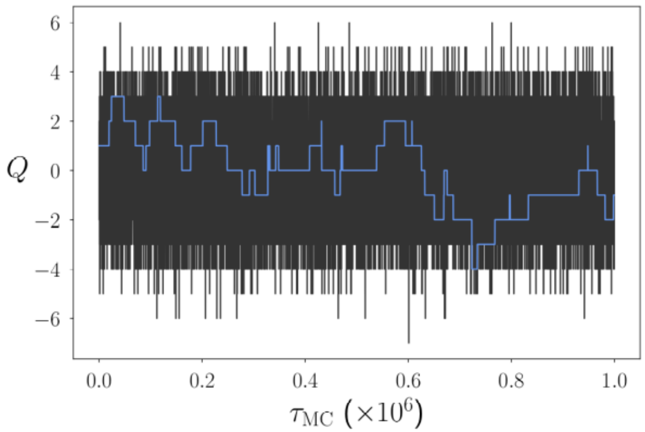
Recap

- wHMC samples faster than HMC the different topological sectors

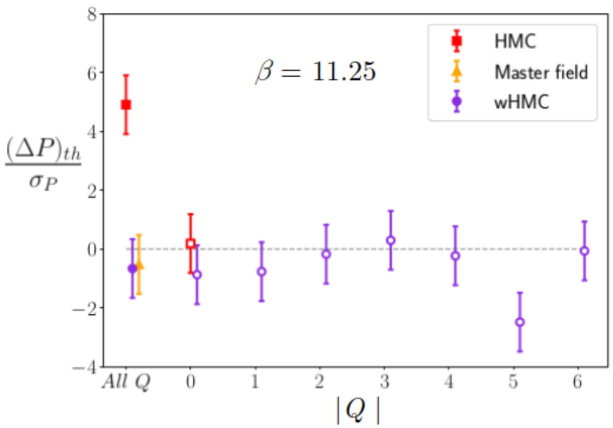


Recap

☆ wHMC samples faster than HMC the different topological sectors

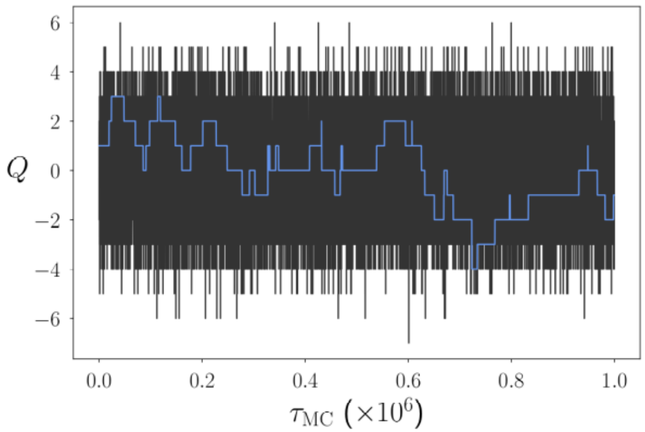


☆ HMC samples correctly within each topological sector, but is biased in the average over all Qs.



Recap

- wHMC samples faster than HMC the different topological sectors



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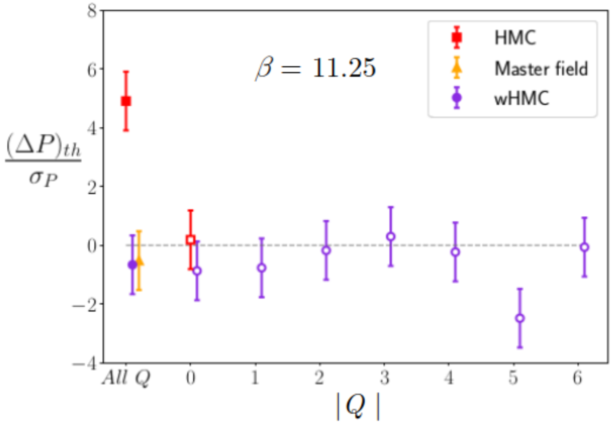
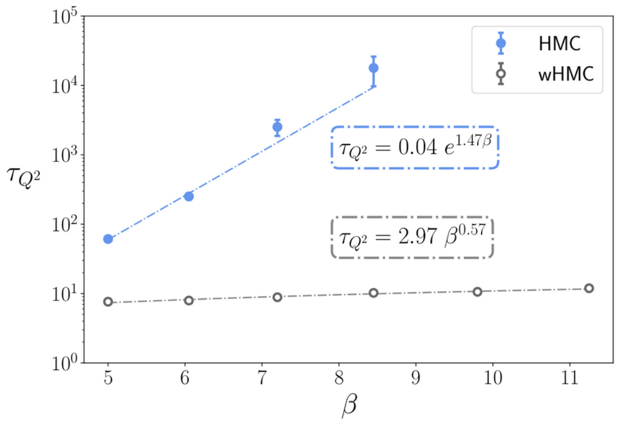


- Autocorrelations increase exponentially for HMC, and with $\sqrt{\beta}$ for wHMC.



Adding fermions: $N_f = 2$

- Partition function without fermions:

$$\mathcal{Z} = \int DU e^{-S[U]}$$

- Adding two dynamical, degenerate fermions we get the determinant of the Dirac operator

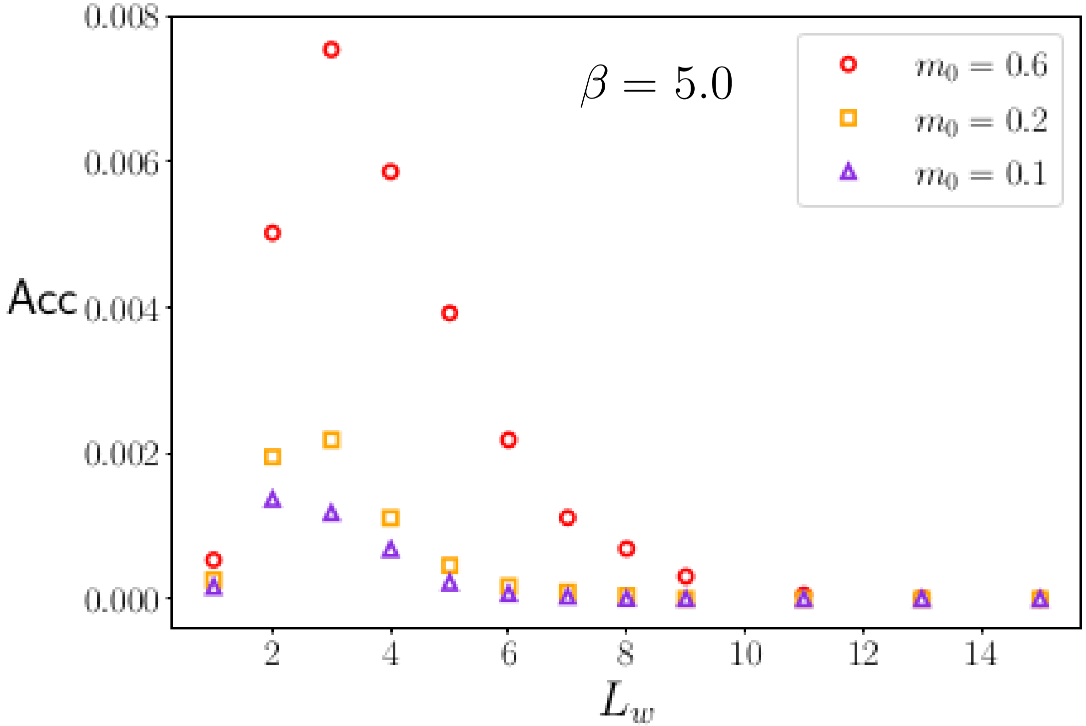
$$\mathcal{Z} = \int \mathcal{D}U e^{-S[U]} \det\left[DD^\dagger\right] = \int \mathcal{D}U\mathcal{D}\phi \; e^{-S[U]-\phi^\dagger(DD^\dagger)^{-1}\phi}$$

- We evaluate the determinant stochastically using a pseudofermion field

- The Dirac operator D is local, but the inverse is highly non-local

  ↳ Even a small transformation can change a lot the action, so we expect the acceptance to decrease

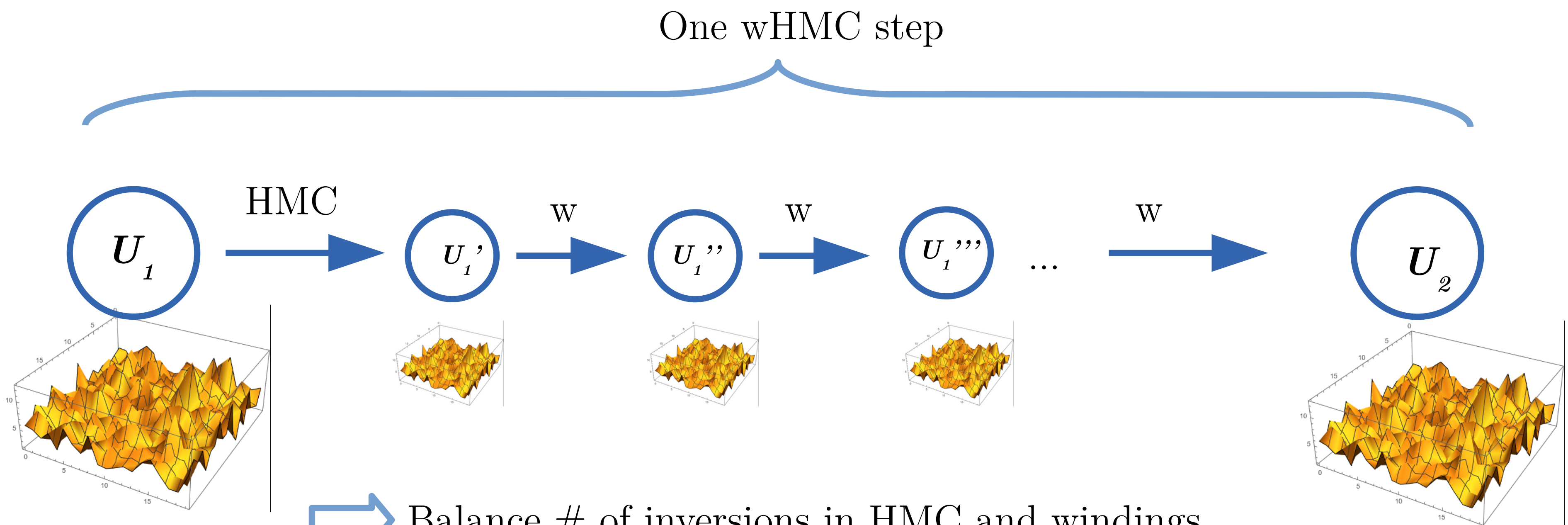
$N_f = 2$



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

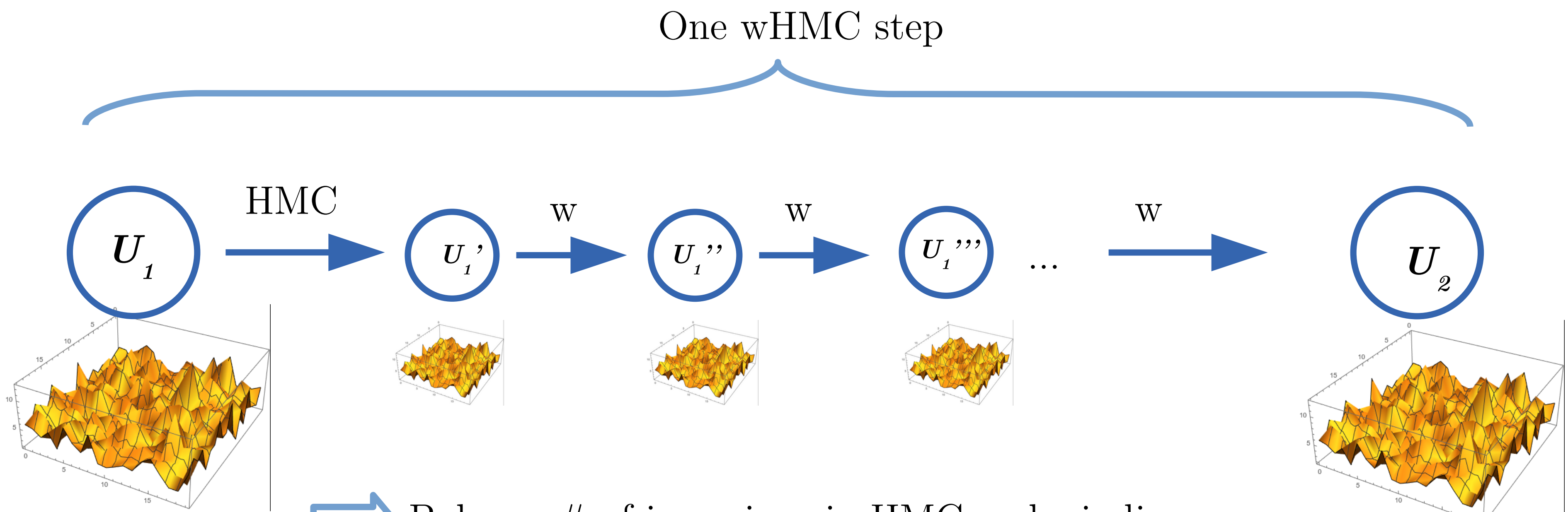
⮱ perform several windings per step

$N_f = 2$



⇨ Balance # of inversions in HMC and windings
(tune the amount of time devoted to HMC evolution and to winding transformations)

$N_f = 2$



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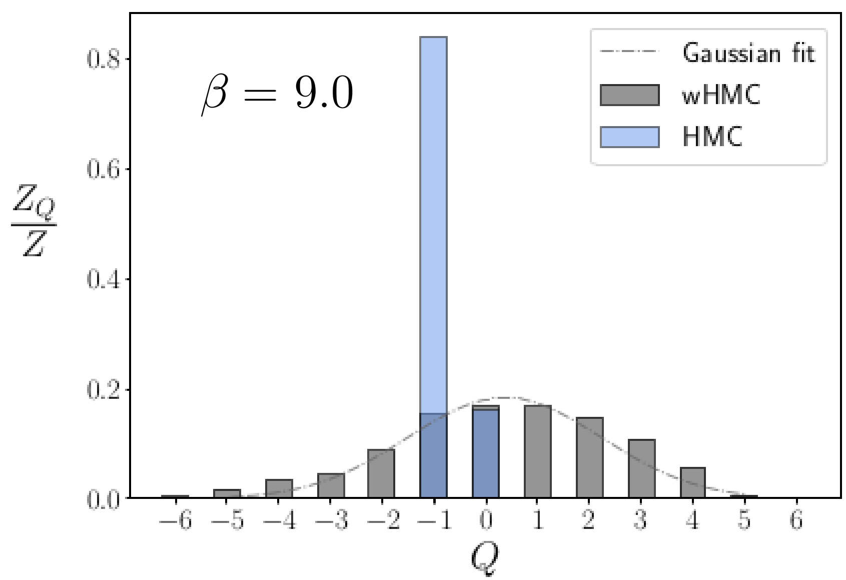
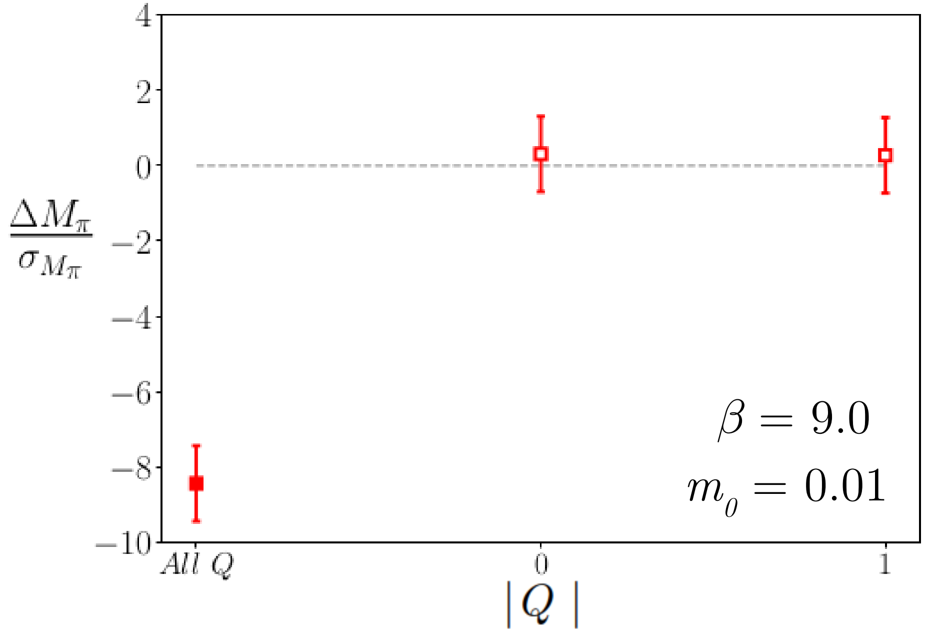


☆ At equivalent computational costs, wHMC is still able to sample all relevant topological sectors

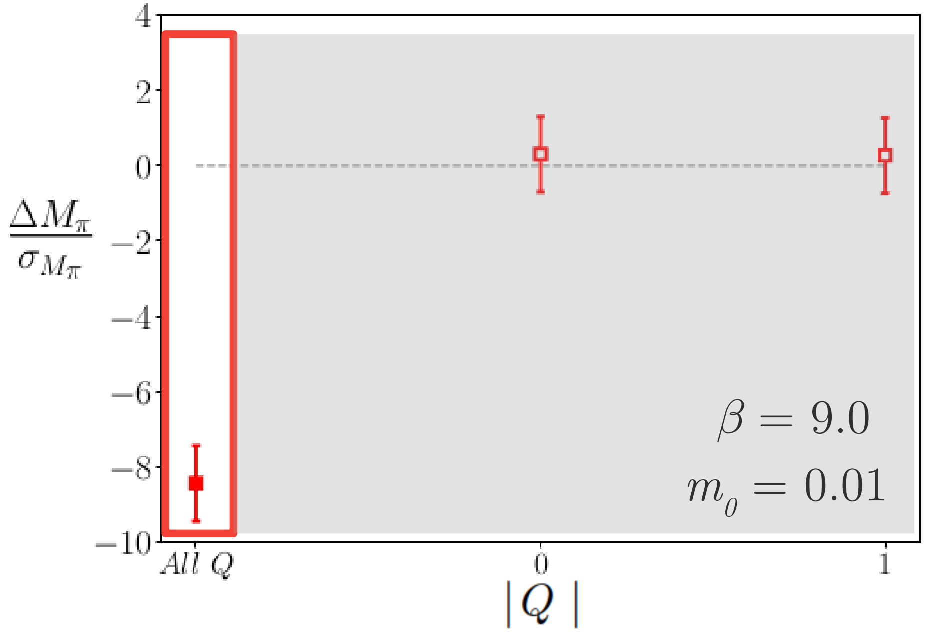
$N_f = 2$ results

Pion Mass discrepancy between wHMC and HMC



$N_f = 2$ results

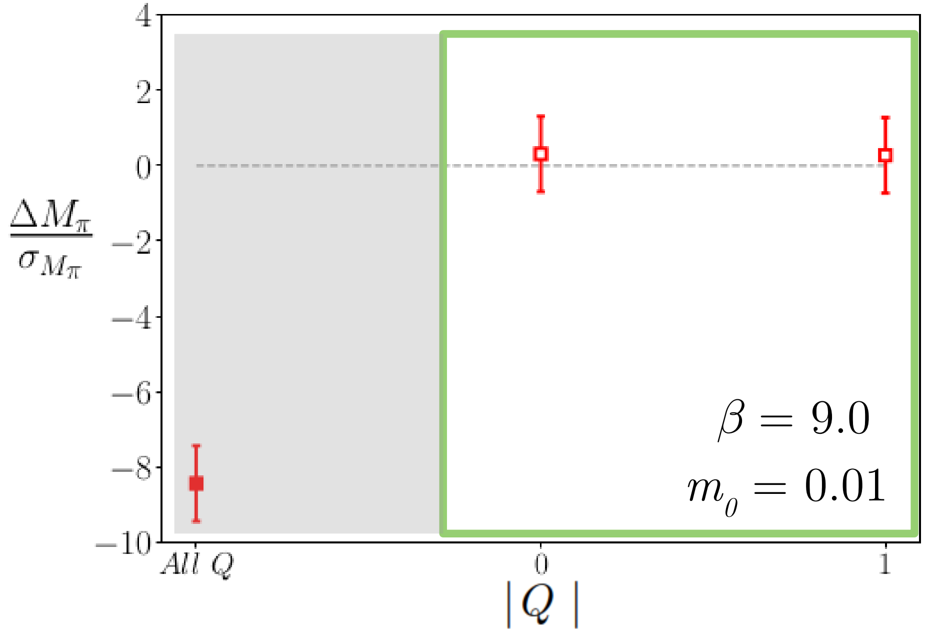
Pion Mass discrepancy between wHMC and HMC



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

$N_f = 2$ results

Pion Mass discrepancy between wHMC and HMC



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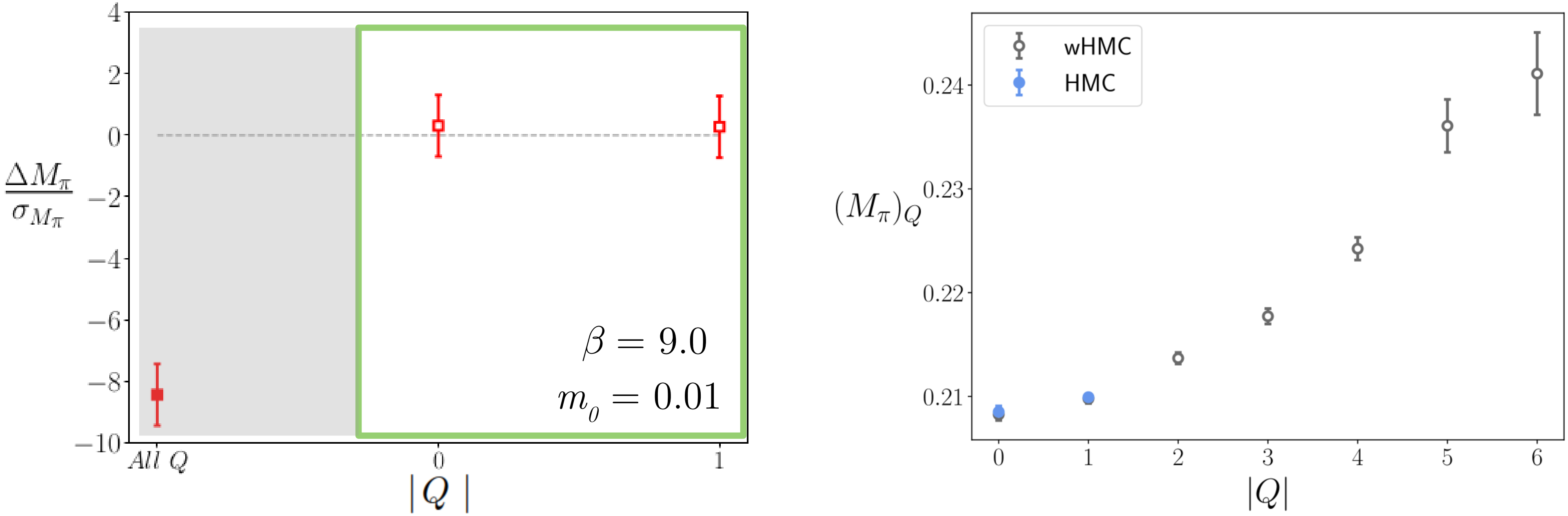
- but samples correctly $Q = 0$ and $Q = 1$

Pion Mass discrepancy between wHMC and HMC



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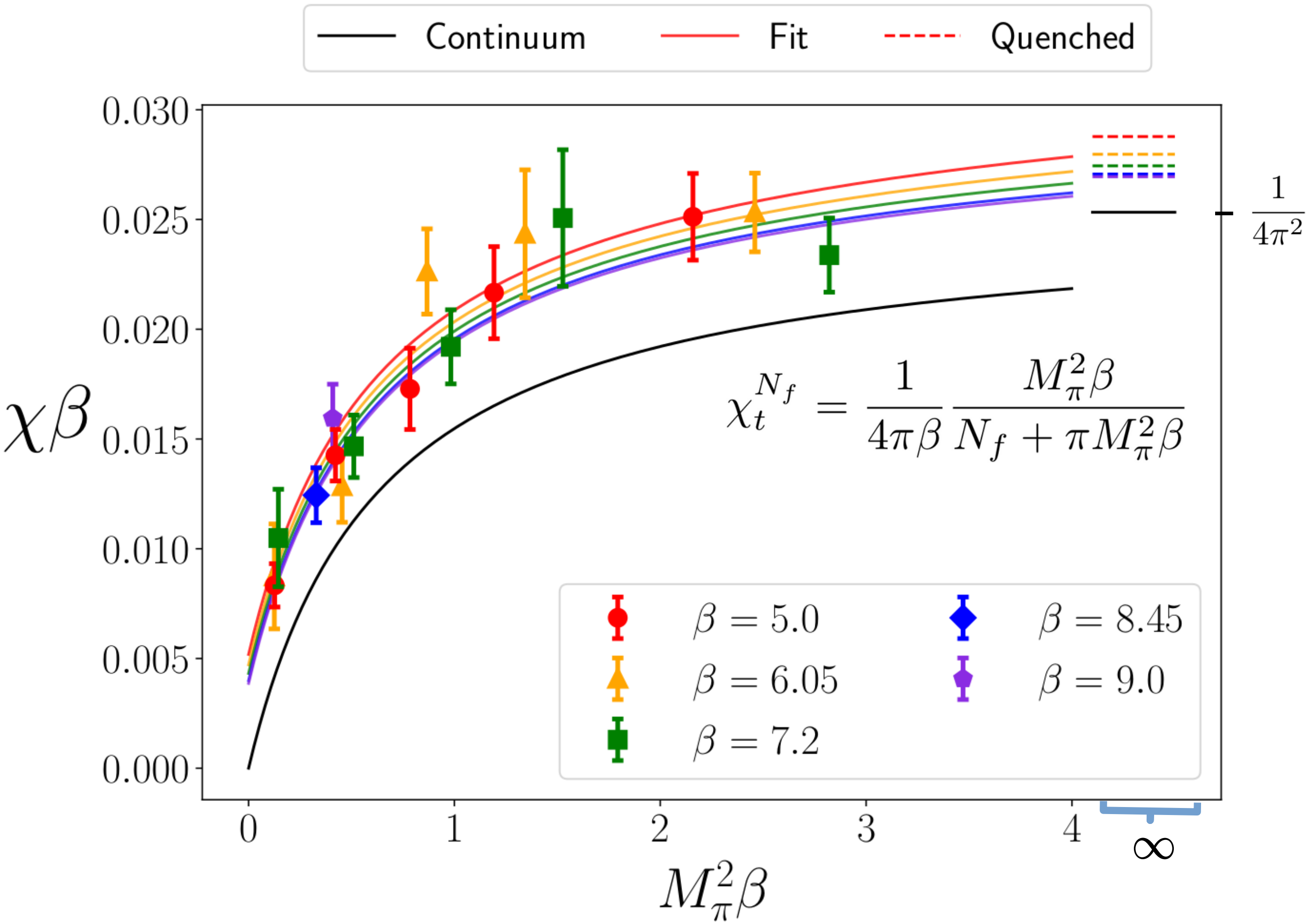
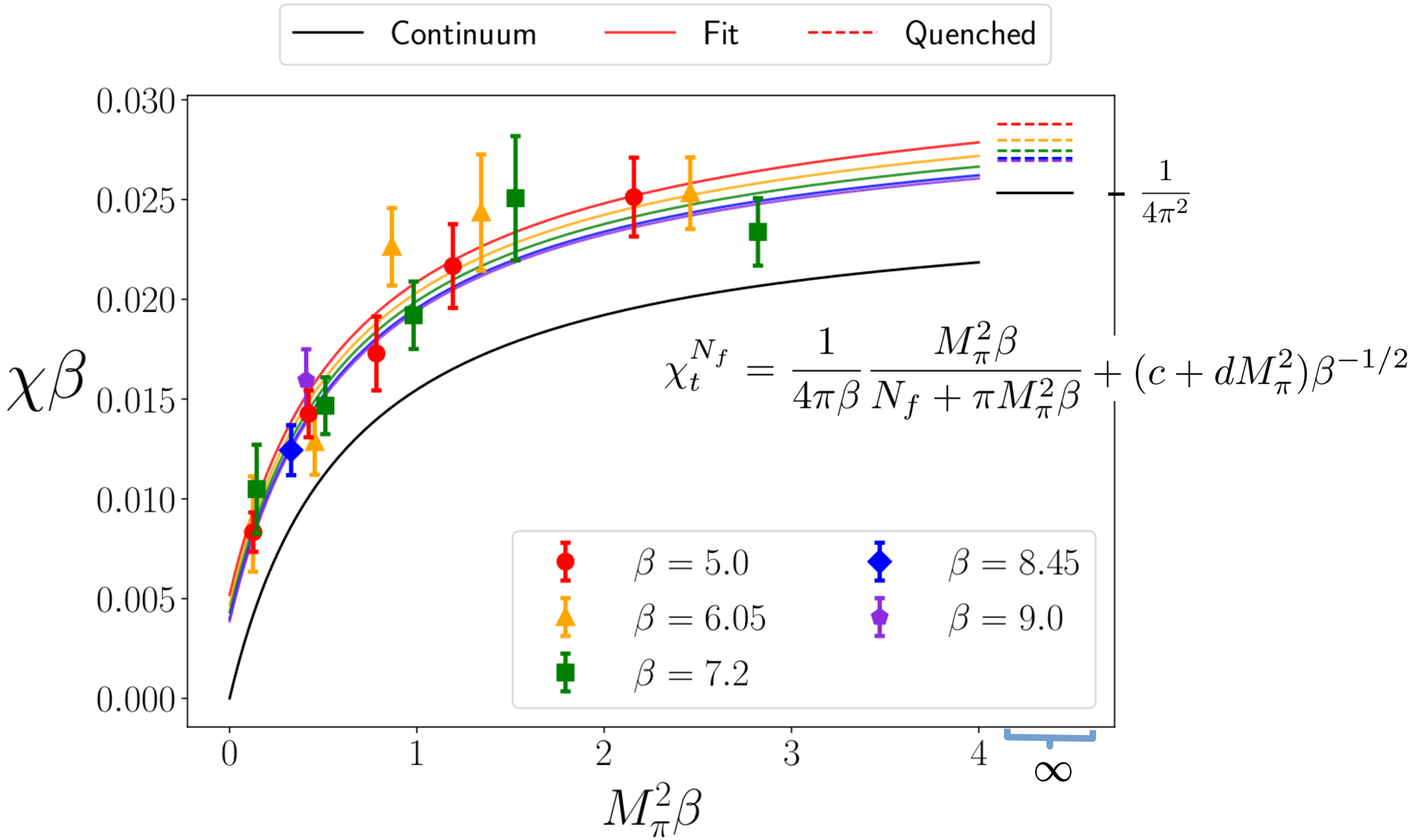
$N_f = 2$ results



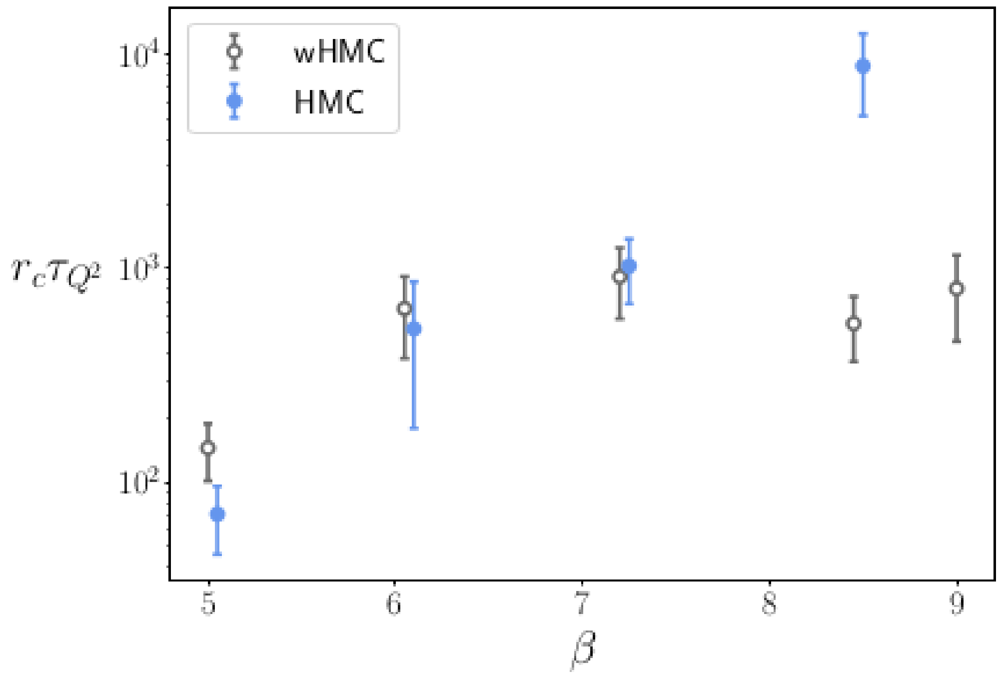
Good agreement with chiral and quenched limits

$N_f = 2$ results



☆ Good agreement with chiral and quenched limits

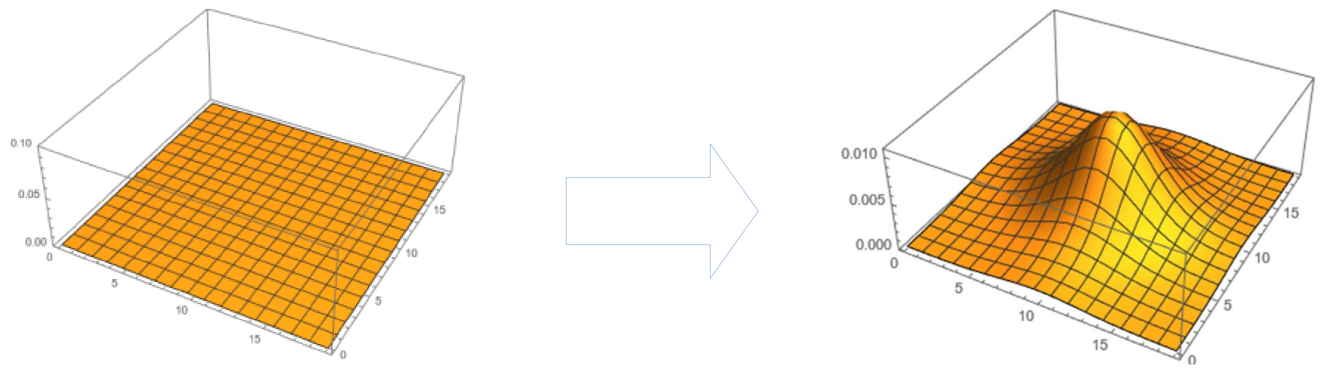
$N_f = 2$ results: scaling with a



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

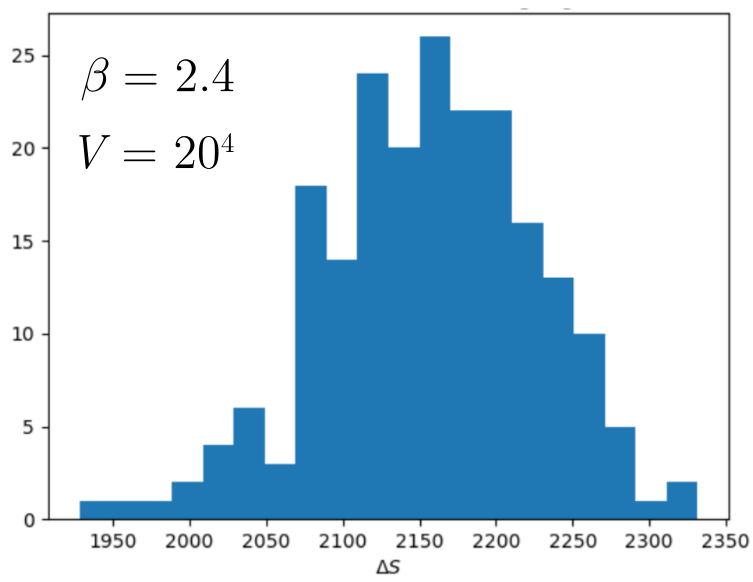
Generalization to SU(2) in 4D

winding transformation



$Q = 0$ $\qquad$ $Q = 1$

- One can generalize naively the winding transformation to SU(2) gauge theory



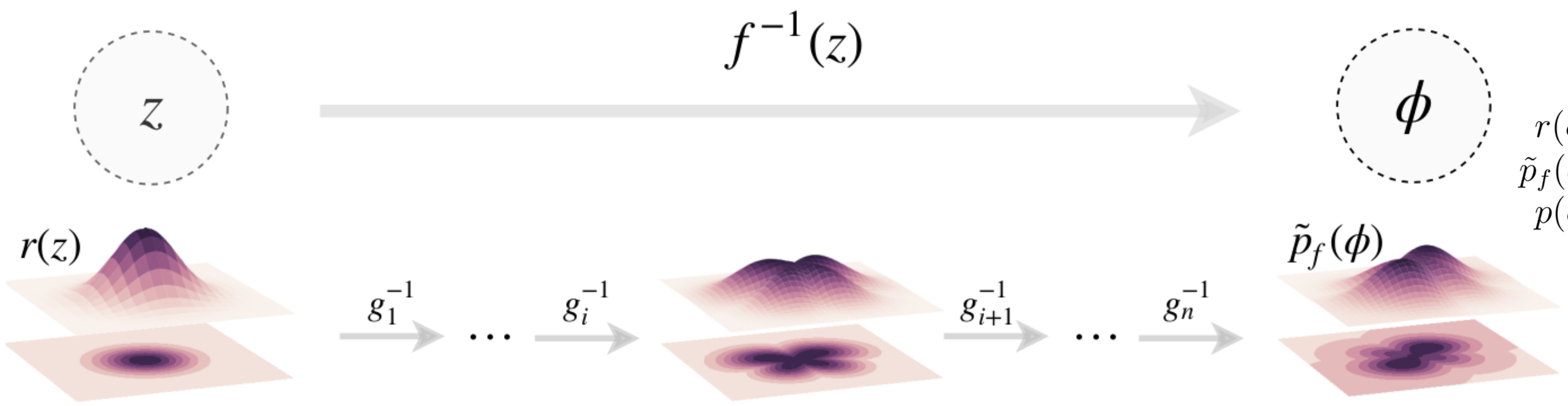
- However, only found poor acceptances

  ⇒ need to explore new ideas!

Future plans: equivariant flows

Luigi del Debbio
Richard Kenway
Joe Marsh Rossney

David Albandea
Pilar Hernández
Alberto Ramos



$r(\phi)$: input distribution
$\tilde{p}_f(\phi)$: output distribution
$p(\phi)$: target distribution

(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

f(z) is a network trained to minimize the KL divergence: $D_{\mathrm{KL}}(\tilde{p}_\theta \,||\, p) = \int \mathcal{D}\phi \, \tilde{p}_\theta(\phi) \log \frac{\tilde{p}_\theta(\phi)}{p(\phi)}$

Can equivariant flows be helpful as Lüscher's trivializing flows for HMC?

Lüscher, M. Trivializing Maps, the Wilson Flow and the HMC Algorithm. Commun. Math. Phys. 293, 899 (2010)

Summary

- 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