

Lattice QCD on Non-Orientable Manifolds

Part I

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P-Boundaries

Quenched Data

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Topological Freezing

Topological charge is the integral

$$Q = \int_{\mathcal{M}} d^4x q(x)$$

over the topological charge density

$$q(x) = \frac{1}{4\pi^2} \epsilon_{\mu\nu\rho\sigma} \text{tr}(F_{\mu\nu}(x) F_{\rho\sigma}(x))$$

- **discretized** in finite volume on $\mathcal{M} = \mathbb{T}^4$
- **topological** invariant
- MC algorithms with small "step" size in field space:
problem for **ergodicity**, diverging τ_{int} of **slow** modes

Ideas

Why introduce non-orientable manifolds?

- Topological freezing
 - topological structure of field space
 - topological charge Q
 - pseudoscalar
 - orientation

Several Ansätze in literature, e.g.

- subvolumes [Brower:2014bqa]
- metadynamics [Laio:2015era]
- multiscale equilibration [Endres:2015yca]
- open boundary conditions [Luscher:2011kk]

Open Boundaries

- Topological structure of the field space depends on **gauge group** and **space-time**

Open Boundaries

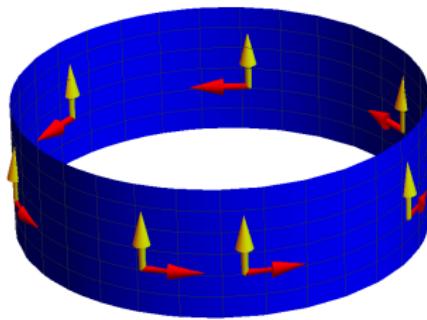
- change topology of **space-time** and **field space**
→ charge is not discretized
- break translational invariance strongly at the boundaries
→ local structure of **space-time**, local QFT is changed
→ effect propagates into the bulk

Alternative:

- different change in the topology of **space-time** without any local changes of **space-time**

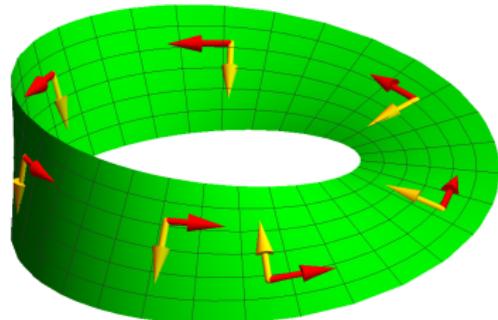
Orientability

orientable:



The One Ring

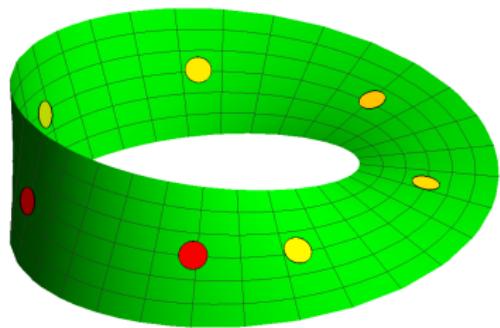
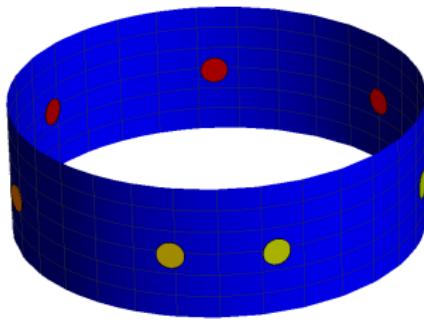
non-orientable:



The Möbius Strip

Topological Charge and Orientability

$q(x)$ is a pseudoscalar density



orientable roundtrip:
no effect on charge

non-orientable roundtrip:
changes sign of charge

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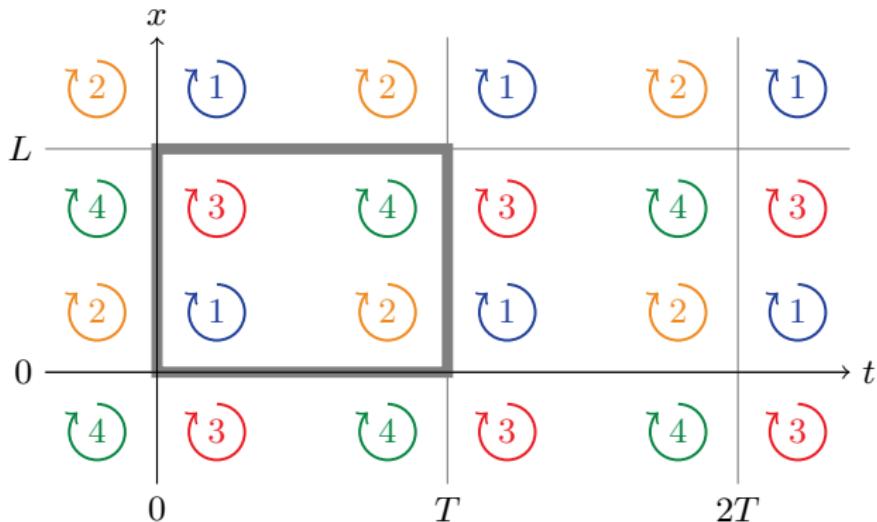
P-Boundaries

- Replace the periodic boundary conditions in one direction by P-periodic boundaries
- i.e. implement an additional parity transformation P on all fields in the boundary condition

Result:

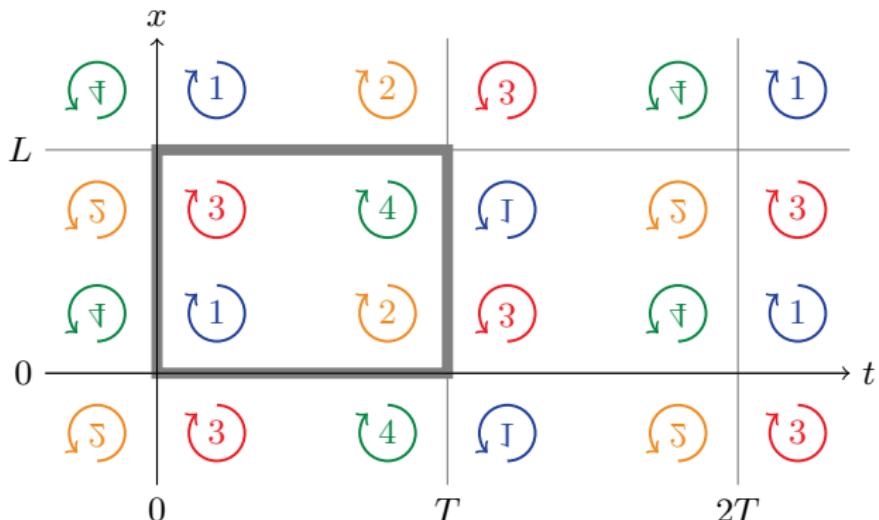
- Topology of space-time changes
→ topology of field space changes
- Charge is P -odd, continuous translation in P -direction
→ charge cannot be discretized
- No hard local breaking of translation invariance

Universal Cover – Torus



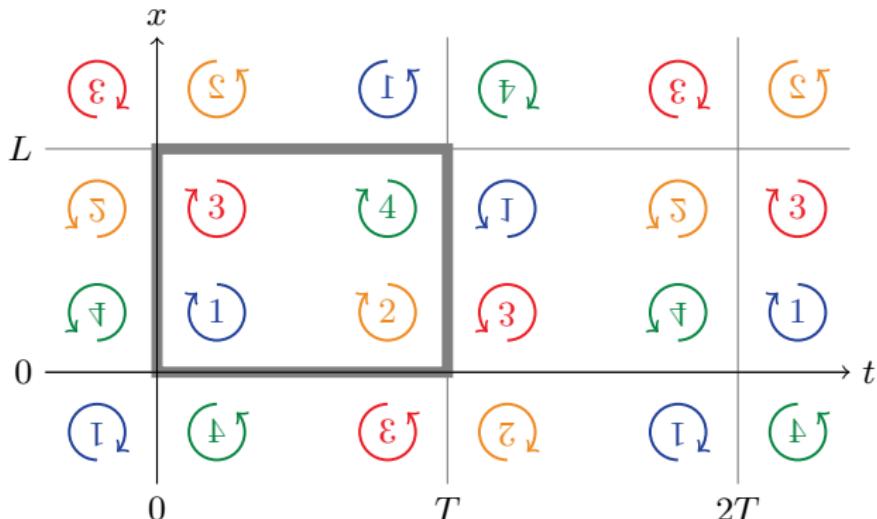
No breaking of translational invariance

Universal Cover – P-periodic in t



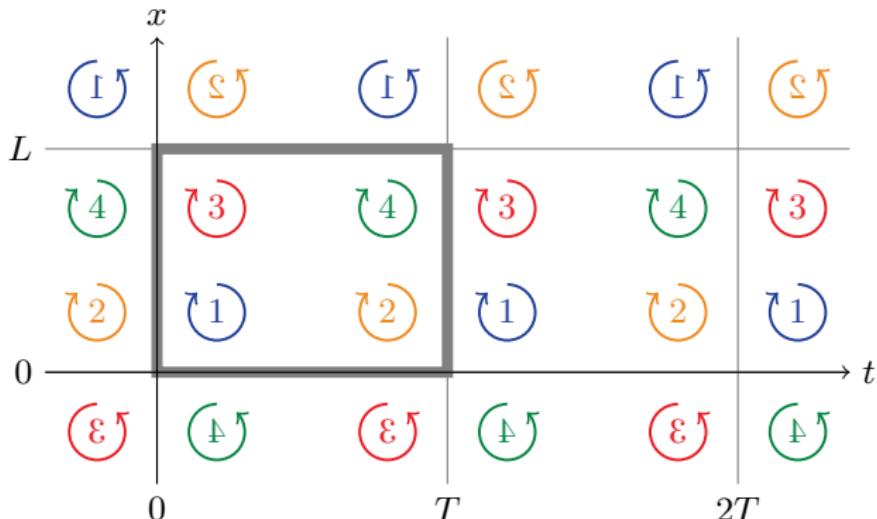
No hard local breaking of translational invariance

Universal Cover – P-periodic in t and x



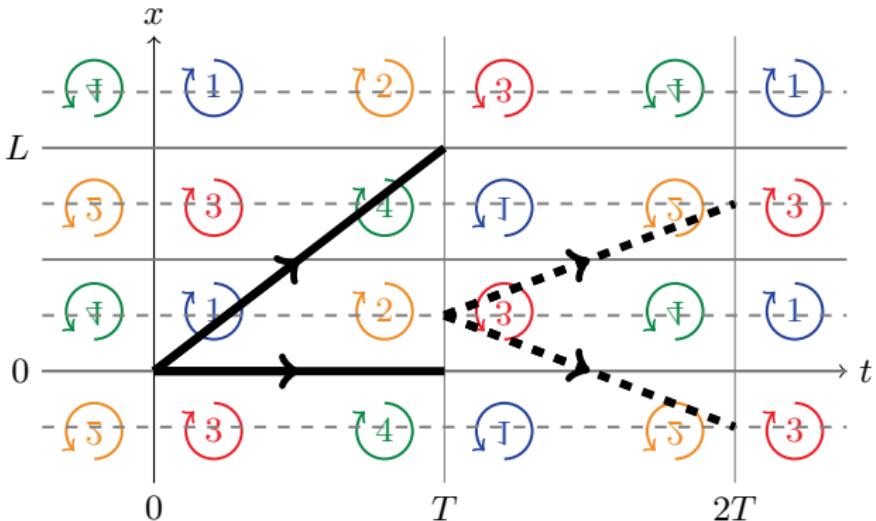
Hard local breaking of translational invariance

Universal Cover – P-periodic in x



No hard local breaking of translational invariance

Universal Cover – Soft Breaking



Soft breaking of translational invariance in x
exponentially suppressed (similar to C^\star : [Lucini:2015hfa])

P-Boundaries: Actual Implementation (Pure Gauge)

- Easier to implement in parallel than P transformation:
Reflection R_x of single coordinate x
- $R_x \equiv P \times \text{rotation by } \pi$

$$U_x(x, y, z, t + T) = U_x^\dagger(L - x - 1, y, z, t),$$
$$U_i(x, y, z, t + T) = U_i(L - x, y, z, t)$$

for $i = y, z, t$. In the other three directions we keep the usual periodic boundary condition.

P-Boundaries: Implementation Options

Reflection of direction x :

- 1 Local (vectorization) \times direction (shuffle, permute)
 - 2 Change in the communication pattern
- ⇒ Implementation **without impact on performance** possible

Multiple P-periodic directions:

- reflect x direction for translations in t , y , z direction
- **more topological charge dynamics**
- **no additional cost**

Integration on Non-Orientable Manifolds

- No global volume form to define integration
- But volume element
 - integrate scalar densities
 - cannot integrate pseudoscalar density $q(x)$

Workaround using local volume form:

Define a total charge Q_m on a maximal oriented submanifold

$$Q_m = \int_0^T dt \int d^3\mathbf{x} q(\mathbf{x})$$

(same expression for open boundaries)

Drop index " $_m$ ": $Q := Q_m$

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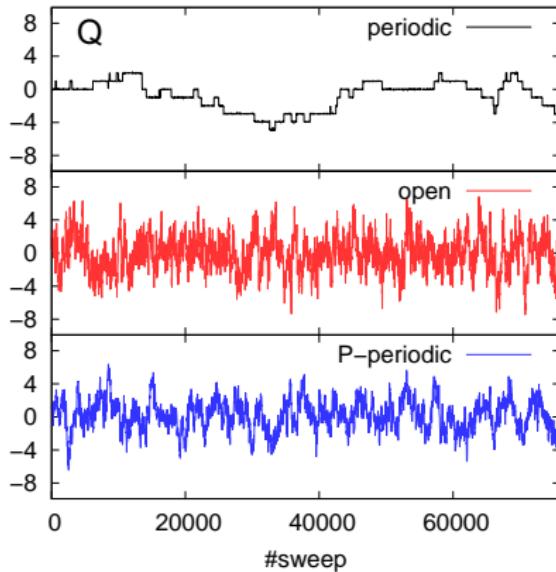
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History of the topological charge Q

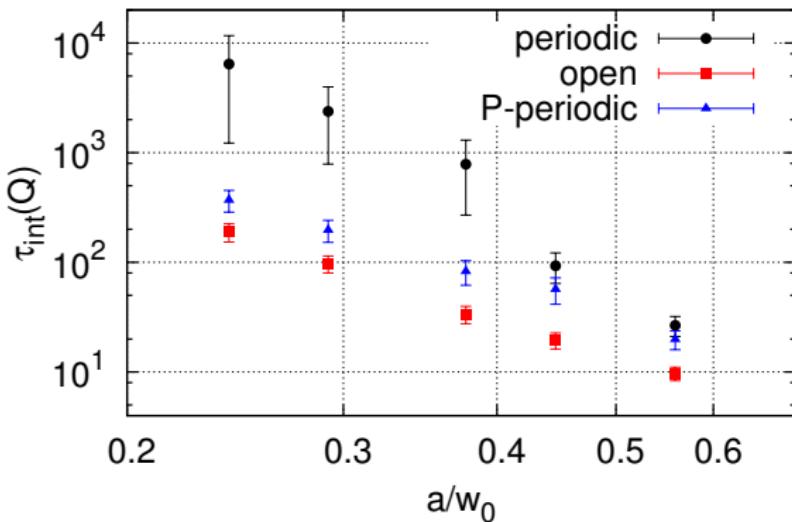


$\beta = 5.1$, lattice spacing $a = 0.040$ fm, and box size 1.6 fm.

Claims

- 1 scaling of $\tau_{\text{int}}(Q)$ with lattice spacing is improved

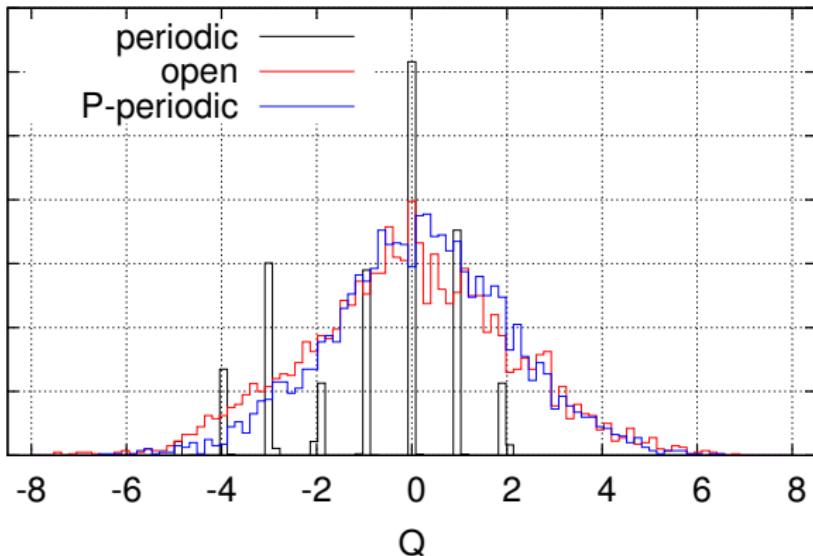
Integrated autocorrelation time



Claims

- 1 scaling of $\tau_{\text{int}}(Q)$ with lattice spacing is improved
better than periodic boundaries
similar to open boundaries
- 2 Q is not quantized

Histogram of the topological charge

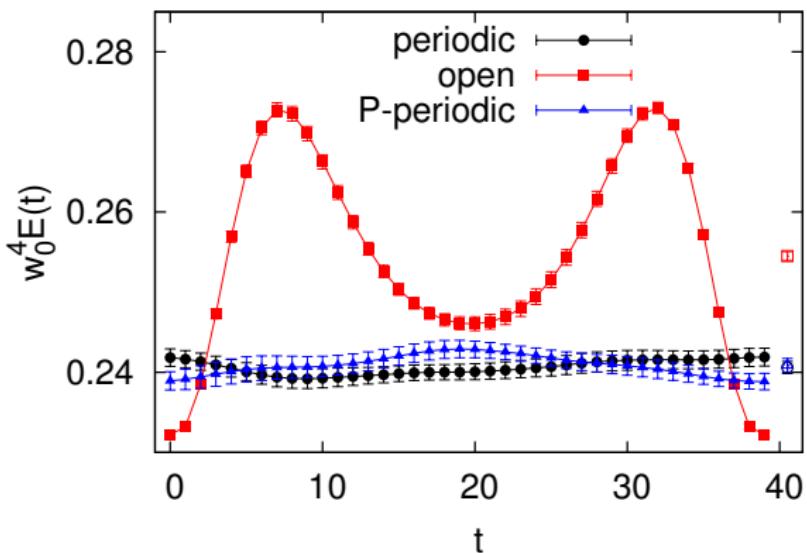


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different from periodic boundaries
similar to open boundaries
- 3 breaking of translational symmetry is suppressed

Time slice averaged action density

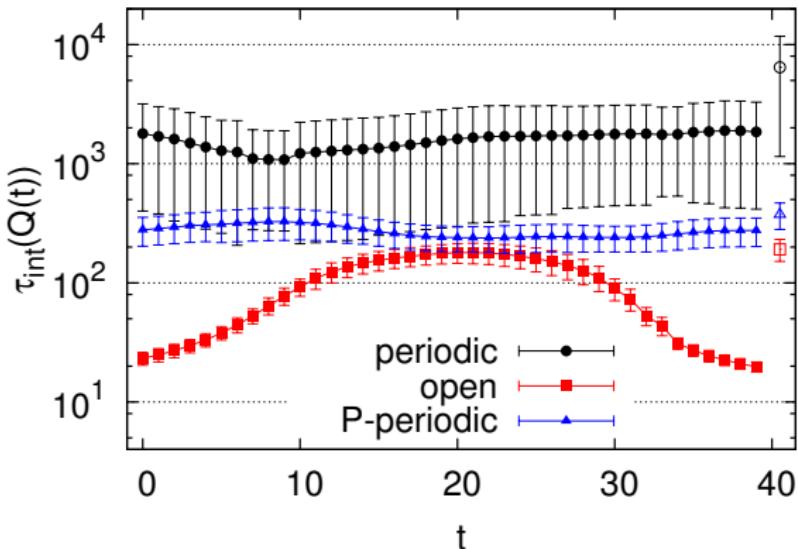


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different from periodic boundaries
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similar to periodic boundaries
better than open boundaries

Time slice autocorrelation time



$\beta = 5.1$, lattice spacing $a = 0.040$ fm, and box size 1.6 fm.

Instanton picture

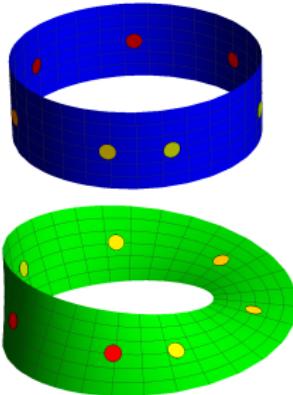
Observables are well-behaved

→ classical field space is connected? **NO!**

- Instantons reflect sectors: $Q = N_+ - N_-$
- Instanton dynamics connects sectors:
pair-creation, propagation + lattice artefacts

Torus: $Q = N_+ - N_-$ conserved

→ ∞ sectors



Open: $N_+ \pm N_-$ not well defined

→ **1** sector

P: $N_+ + N_-$ conserved mod 2

→ **2** sectors!

Ideas for the two Sectors

Only two sectors

- 2 are easier to sample than $\infty \rightarrow$ reach higher β

Equivalence of the sectors? For 2D $U(1)$

- \exists mapping between sectors 0 and 1
- leaving action and measure invariant

Relative weight of the sectors

- run a frozen stream for sector 0 and 1 \rightarrow average
 - Identical weight of the sectors?
 - Estimate from topological susceptibility?
 - Integrate up relative weight from betas with tunneling
 - Unknown weight \Rightarrow systematic error

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Open issues:

- two remaining **sectors** of classical field space
- include fermions: **spinors** on non-orientable manifolds
⇒ construction in **Balints talk**

Non-orientable manifolds are **useful** and **interesting**:

- improve topological autocorrelations
⇒ **similar** to open boundaries
- suppressed breaking of translational symmetry
⇒ **better** than open boundaries
- new toy in lattice QCD toolbox ⇒ **new opportunities**



Diffusion Model

Describe autocorrelations in simulation time
[McGlynn, Mawhinney, PRD 90 (2014) 7]

$$C(t, t_0, \tau) \equiv \langle Q(t + t_0, \tau_0 + \tau) Q(t_0, \tau_0) \rangle$$

$$\frac{\partial}{\partial \tau} C(t, t_0, \tau) = D \frac{\partial^2}{\partial t^2} C(t, t_0, \tau) - \frac{1}{\tau_{\text{tunn}}} C(t, t_0, \tau),$$

- topological charge $Q(t, \tau)$ on a time slice t at simulation time τ
- diffusion constant D
- timescale for topological charge tunneling τ_{tunn}

Diffusion Model

- Solutions determine integrated autocorrelation time
- Solutions determined by symmetry of boundaries

Boundary	periodicity	τ_{int}
Torus	$C(t + T, t_0, \tau) = C(t, t_0, \tau)$	$\propto \tau_{\text{tunn}}$
P	$C(t + T, t_0, \tau) = -C(t, t_0, \tau)$	$\propto D^{-1}$
Open $t_0 = \frac{T}{2}$	" $C(t + T, \frac{T}{2}, \tau) = -C(t, \frac{T}{2}, \tau)$ "	$\propto D^{-1}$

- Same τ_{int} for P and (middle of) open
- Only torus is dependent on τ_{tunn} for small τ_{tunn}

Quenched Parameters

- Symanzik gauge action
- sweeps of one heatbath plus four overrelaxation
- fixed physical size of $L = T \sim 2.27/T_c$

L	β	w_0	$a[\text{fm}]$	n_{sweep}
16	4.42466	1.79	0.093	2×4001
20	4.57857	2.24	0.075	3×4001
24	4.70965	2.65	0.063	4×4001
32	4.92555	3.43	0.049	10×4001
40	5.1	4.13	0.040	19×4001

Remarks on Observables

Topological Susceptibility on P-boundaries:

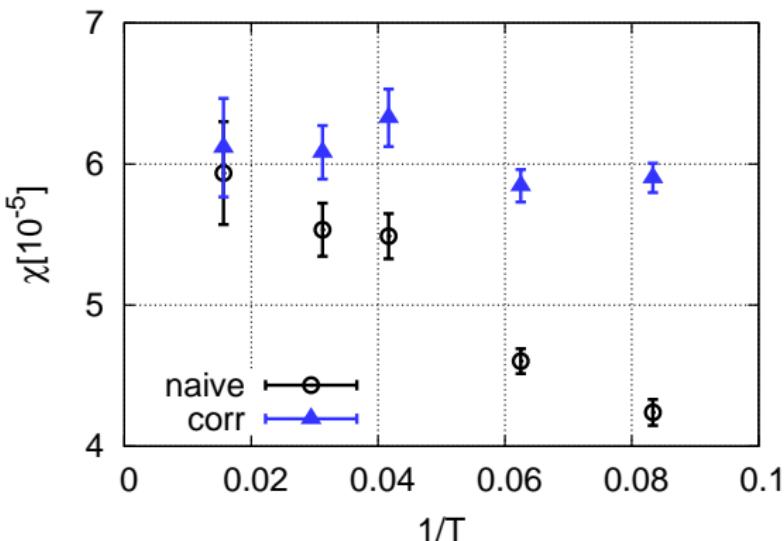
$$\chi = \int_{\mathcal{M}} d^4x \langle q(0)q(x) \rangle \neq \frac{1}{V_4} \langle Q^2 \rangle$$

due to missing translational symmetry of $q(x)$
(similar to subvolume method)

Alternative:

- evaluate $\chi = \int_0^T dt \int d^3x \langle q(\mathbf{0}, T/2)q(\mathbf{x}, t) \rangle$ directly
⇒ reduced finite volume errors

Observables: FV dependence



$\beta = 4.42466$, lattice spacing $a = 0.093$ fm,
fixed spatial size L , only temporal size T changes