Lattice QCD on Non-Orientable Manifolds

Part I

[1512.06804]

July 24, 2016 | Simon Mages | Bálint C. Tóth Szabolcs Borsányi Zoltán Fodor Sándor D. Katz Kálmán K. Szabó

Outline

Introduction

P-Boundaries

Quenched Data

Outlook

Outline

Topological Freezing

Topological charge is the integral

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

over the topological charge density

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

- 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
  - $\rightarrow$ topological structure of field space
  - $\rightarrow$ topological charge Q
  - $\rightarrow$ pseudoscalar
  - $\rightarrow$ orientation

Several Ansätze in literature, e.g.

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

[Mo 14:15 Bietenholz]
[Tu 10:45 Endres]
[Tu 15:40 Toussaint]
[Tu 19:10 Sanfillipo]
[Fr 14:20 Garcia Vera]

Open Boundaries

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

Open Boundaries

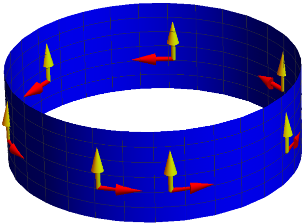
- change topology of space-time and field space
  $\rightarrow$ charge is not discretized
- break translational invariance strongly at the boundaries
  $\rightarrow$ local structure of space-time, local QFT is changed
  $\rightarrow$ effect propagates into the bulk

Alternative:

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

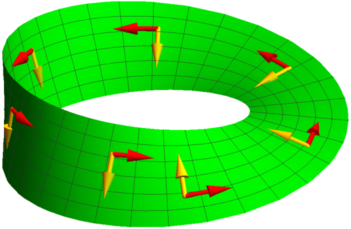
Orientability

orientable:



The One Ring

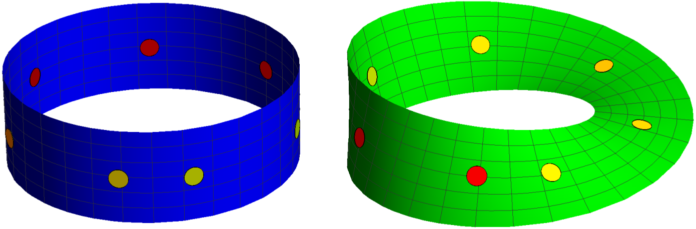
non-orientable:



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

Outline

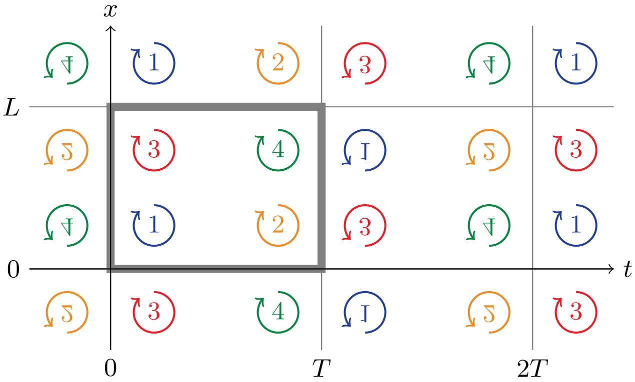
P-Boundaries

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

Construction on the Universal Cover



Integration on Non-Orientable Manifolds

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

Workaround using local volume form:

Define a total charge Q_m on a maximal oriented submanifold

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

(same expression for open boundaries)

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

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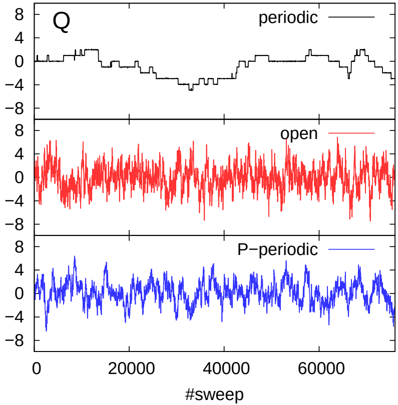
History of the topological charge Q

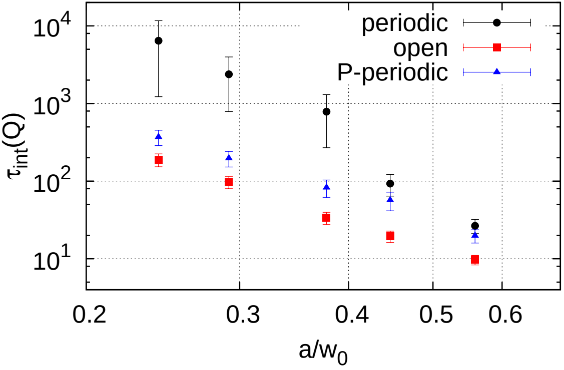


$\beta = 5.1$, lattice spacing $a = 0.040$ fm, and box size 1.6 fm.

Claims

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

Integrated autocorrelation time

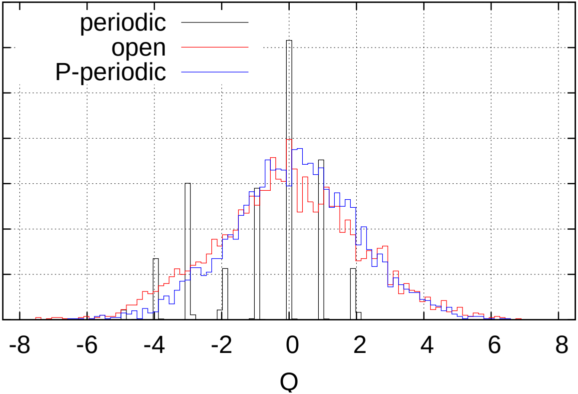


box size 1.6 fm.

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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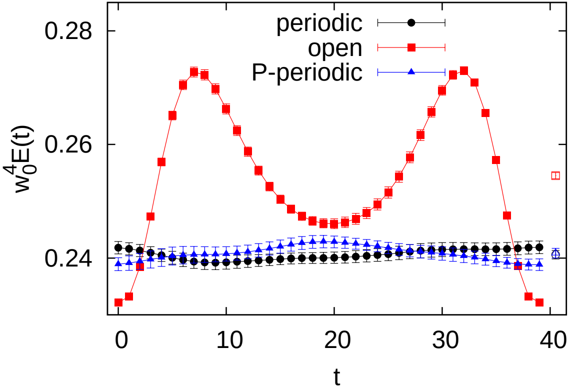
   similar to open boundaries
2. Q is not quantized
   different from periodic boundaries
   similar to open boundaries
3. breaking of translational symmetry is suppressed

Time slice averaged action density



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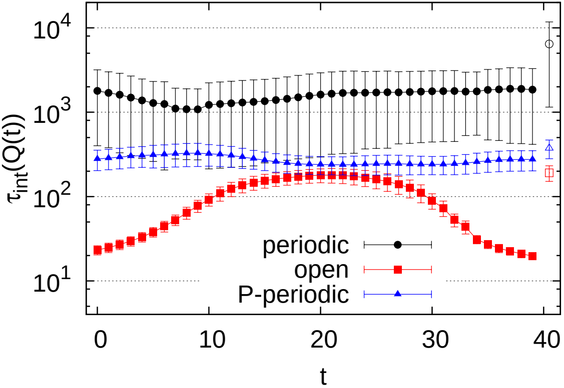
3. breaking of translational symmetry is suppressed
   similar to periodic boundaries
   better than open boundaries

Time slice autocorrelation time



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

Instanton picture

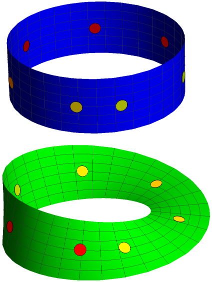
Observables are well-behaved
$\rightarrow$ classical field space is connected? NO!

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

Torus: $Q = N_+ - N_-$ conserved
$\rightarrow \infty$ sectors

Open: $N_+ \pm N_-$ not well defined
$\rightarrow$ 1 sector

P: $N_+ + N_-$ conserved mod 2
$\rightarrow$ 2 sectors!



Outline

Outlook

Open issues:

- two remaining sectors of classical field space
  $\Rightarrow$ more details in Balints talk
- include fermions: spinors on non-orientable manifolds
  $\Rightarrow$ construction in Balints talk

Non-orientable manifolds are useful and interesting:

- improve topological autocorrelations
  $\Rightarrow$ similar to open boundaries
- suppressed breaking of translational symmetry
  $\Rightarrow$ better than open boundaries
- new toy in lattice QCD toolbox $\Rightarrow$ 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}

P-Boundaries: Actual Implementation (Pure Gauge)

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

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

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

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[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:

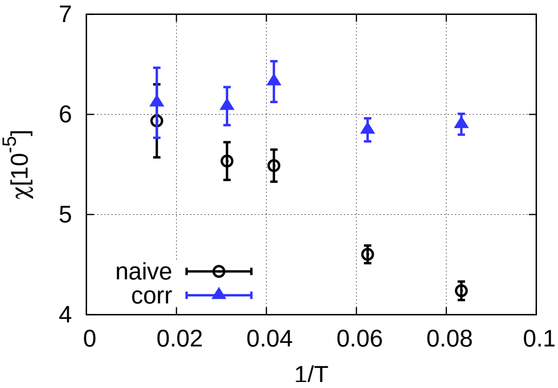
$$\chi = \int_{\mathcal{M}} \mathrm{d}^4 x \langle q(0) q(x) \rangle \neq \frac{1}{V_4} \langle Q^2 \rangle$$

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

Alternative:

- evaluate $\chi = \int_0^T \mathrm{d}t \int \mathrm{d}^3 x \langle q(\mathbf{0}, T/2) q(\mathbf{x}, t) \rangle$ directly
  $\Rightarrow$ 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