Computing the topological susceptibility from fixed topology QCD simulations

Arthur Dromard
In collaboration with: Wolfgang Bietenholz, Krzysztof Cichy and Marc Wagner.

Department of Theoretical Physics
Goethe Universität, Frankfurt am Main

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1 Motivation
   - Topology in QCD
   - Topology freezing problem on the lattice

2 AFHO method
   - Method description
   - Numerical results

3 Slabs method
   - Method description
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**Definition: Topology**

Topology is the study and the classification of objects which are equivalent by continuous deformations. In field theory, you can classify fields by an integer: its topological charge.

**Definition: Topological object**

Non-trivial structures in field configurations, which cannot be removed by continuous deformations, while keeping the action finite (their position can be changed and they can be deformed). They carry the topological charge.
Topology in QCD

- Path integral formalism:

\[ Z = \int DAD\psi D\bar{\psi} e^{-S[A,\bar{\psi},\psi]} \]

- Each \( A_\mu \), has a topological charge \( Q[A] \)

\[ Q[A] = \frac{g^2}{32\pi^2} \int F_{\mu\nu} \tilde{F}_{\mu\nu} \in \mathbb{Z} \]

To take into account topology in your action:

- Action with topological term:

\[ S_E(\theta) = S_E - i\theta \frac{g^2}{32\pi^2} \int F_{\mu\nu} \tilde{F}_{\mu\nu} = S_E - i\theta Q[A] \]

- The P symmetry is lost for \( \theta \neq 0 \)

For QCD: \( \theta_{QCD} \leq 10^{-10} \)
Topological susceptibility in QCD

- The topological susceptibility:

\[ \chi_T = \left. \frac{\partial^2 e_0(\theta)}{\partial \theta^2} \right|_{\theta=0} \neq 0 \]

- Topological susceptibility is particularly important in QCD:
  - example: Witten-Veneziano Formula for the large \( \eta' \)-mass.

**Infinite volume:**

- Topological charge distribution: first approximation:

\[ p(Q) \propto \exp\left(-\frac{Q^2}{2\langle Q^2 \rangle}\right) \]

- And then the topological susceptibility

\[ \chi_T = \frac{\langle Q^2 \rangle}{V} \]
Topology on lattice

- Configurations are produced by Monte-Carlo algorithm
- Proceed to create new configuration by small discrete transformations
  - allow the algorithm to change $Q$
  - can easily compute
    
    $$\chi_T = \frac{\langle Q^2 \rangle}{V}$$

- Smaller lattice spacing $\Rightarrow$ transformations closer to continuous deformations

**Problem:**

- Topology freezes for a too small lattice spacing $a < 0.05\text{fm}$
  [Luscher, Martin JHEP 1008 (2010) 071]

- One can fix the topology in purpose:
  - High quality fermions $\Rightarrow$ Overlap fermions
  - Mixed action, …
Fixed topology simulations problem

- If topology is fixed:

\[ Z_Q = \int \mathcal{D}A \mathcal{D}\psi \mathcal{D}\bar{\psi} \delta_{Q,Q[A]} e^{-S[A,\bar{\psi},\psi]} \]

results will exhibit systematic errors

- Errors are proportional to \(1/\chi_T V\), and their behavior can be calculated as a power series in \(1/\chi_T V\).

\[ \langle O \rangle_Q = \langle O \rangle_{\theta=0} + \frac{1}{2\chi_T V} \left(1 - \frac{Q^2}{\chi_T V}\right) \frac{\partial \langle O \rangle}{\partial^2 \theta} \bigg|_{\theta=0} + \ldots \]


- One cannot determine the topological susceptibility using:

\[ \chi_T = \frac{\langle Q^2 \rangle}{V} \]

Need special methods to extract the topological susceptibility!
Outline

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2-point correlation function

- Fixed topology theory is non-local $\Rightarrow$ no-Hamiltonian exists.
- We can still define a partition function:

$$Z_Q = \int DAD\psi D\bar{\psi}\delta_{Q,Q[A]}e^{-S[A,\bar{\psi},\psi]}$$

- It can be shown that the partition function at fixed topology is the Fourier Transform of the partition function with $\theta$-term:

$$Z_Q = \int d\theta e^{-iQ\theta}Z_\theta$$

- We can apply the same idea on the 2-point correlation functions

$$C_{Q,V}(t) \equiv \frac{1}{Z_{Q,V}} \int DAD\psi D\bar{\psi}\delta_{Q,Q[A]}O^\dagger(t)O(0)e^{-S_E[A,\psi,\bar{\psi}]}$$

where $O$ is a suitable normalized hadron creation operator.
- And it can also be defined as a Fourier transform:

$$C_{Q,V}(t) = \frac{1}{Z_Q} \int d\theta e^{-iQ\theta}Z_\theta C_{\theta,V}(t)$$
Mixing of parity

- Parity $P$ is not a symmetry at $\theta \neq 0$.

- It is not possible to construct two-point correlation functions $\mathcal{C}_{\theta,V}(t)$, where only $P = -$ or $P = +$ states contribute.

\[
\mathcal{C}_{\theta,V}(t) = \left( \alpha_-(\theta, V_s) e^{-M_{H_-}(\theta)t} + \alpha_+(\theta, V_s) e^{-M_{H_+}(\theta)t} \right) e^{-E_0(\theta, V_s)T}
\]

- Similarly $C_{Q,V}(t)$ contains contributions of states both with $P = -$ and $P = +$, since it is the Fourier transform of $\mathcal{C}_{\theta,V}(t)$.

- To perform the Fourier transform, we can approximate it using saddle point approximations and Taylor expansion:

\[
C_{Q,V}(t) = a_{11} e^{-M_{H_-}(0)t} e^{-M^{(2)}_{H_-}(0)t} + \frac{b_{22}}{\chi_t V} e^{-M_{H_+}(0)t} e^{-M^{(2)}_{H_+}(0)t}
\]

\[
C_{Q,V}(t) = \frac{a_{22}}{\chi_t V} e^{-M_{H_-}(0)t} e^{-M^{(2)}_{H_-}(0)t} + b_{22} e^{-M_{H_+}(0)t} e^{-M^{(2)}_{H_+}(0)t}
\]
This can be applied for the following correlators: $\langle q(t)q(0)\rangle$ which has the vacuum as ground state and the $\eta$-meson as parity partner:

$$\langle q(t)q(0)\rangle_{Q,V} \thicksim \frac{\alpha}{\chi_t V} + \ldots$$

Using Ward identities to compute the coefficient, one can prove that:

$$\langle q(t)q(0)\rangle_{Q,V} \thicksim \frac{\chi_t}{V} \left(1 - \frac{Q^2}{\chi_t V}\right) + O\left(\frac{1}{\chi_t^2 V^2}, e^{-m_\eta t}\right)$$


From this formula, a simple method exists to extract the topological susceptibility:

1. Compute the $\langle q(t)q(0)\rangle_{Q,V}$ for one topological sector,
2. For large $t$, fit a constant value,
3. Extract the topological susceptibility knowing $V$ and $Q$

This can be applied for only one volume and only one topological charge.
The configurations are generated by the ETMC code, with Twisted Mass Wilson action and dynamical $u/d$ quarks

Set-up:

- $a \approx 0.079\text{fm}$
- $m_\pi \approx 650\text{MeV}$
- Volume: $16^3 \times 32$
- Number of configurations: 10000

- $|Q|=0 : O(1000)$
- $|Q|=1 : O(1500)$
- $|Q|=2 : O(1300)$

Topological charge computation

- Field definition with clover term
- Smoothing: Gradient Flow
Numerical results

\[ \langle q(t)q(0) \rangle_{Q,V} \approx -\frac{\chi_t}{V} \left( 1 - \frac{Q^2}{\chi_t V} \right) \]
Numerical results

- Numerical results

| $\chi_t \times 10^5$ | $|Q| = 0$ | $|Q| = 1$ | $|Q| = 2$ |
|---------------------|-----------|-----------|-----------|
| unfixed topology    |           | 7.76(20)  |           |
| AFHO (fit 1 sector) | 8.30(45)  | 7.56(34)  | 7.42(37)  |
| AFHO (fit all sectors) |         | 7.69(22)  |           |

- All the results are in agreement!

- The influence of the gradient flow:
  1. Reducing the statistical errors,
  2. Reducing the size of the plateau.

- Drawback of the method:
  - The amplitude of the signal is decreasing as $1/V$,
    - difficult to get precise results for large volume.
  - Need to have $\frac{Q^2}{\chi_t V} < 1$.  

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Theoretical part

- Assuming a Gaussian probability of the topological charge distribution:
  \[ p(Q) \propto \exp(-Q^2/(2\chi_t V)) \]

- We can consider a sub-volume \(xV\), with \(x \in [0:1]\)

  \[ p(q)p(Q-q)|_{xV} \propto \exp\left(-\frac{q^2}{2\chi_t Vx}\right) \times \exp\left(-\frac{(Q-q)^2}{2\chi_t V(1-x)}\right) \]

  with \(q\) being the topological charge on the volume \((xV)\) that we considered.
  (not an integer)

  - You can define: \(q' = q - xQ\).

  \[ p(q)p(Q-q)|_{xV} \propto \exp\left(-\frac{q'^2}{2\chi_t Vx(1-x)}\right) \]

  - It follows:

    \[ \langle q'^2 \rangle = \chi_t Vx(1-x) \]

  - One can calculate \(\langle q'^2 \rangle\) for \(x \in [0:1]\) and fit the parabola to obtain the topological susceptibility.
\[ \langle q'^2 \rangle = \chi_t V x (1 - x) \]
Numerical Results (2)

- The deviation from a parabola is due to the smoothing process (needs to be better understood).
  - fitting is still possible in intermediate value of $x$!
- Numerical results

| $\chi_t \times 10^5$ | $|Q| = 0$ | $|Q| = 1$ | $|Q| = 2$ |
|----------------------|-----------|-----------|-----------|
| unfixed topology     |           | 7.76(20)  |           |
| Slabs (fit 1 sector) | 8.23(30)  | 7.72(21)  | 7.38(39)  |
| Slabs (fit all sectors) |     | 7.63(14)  |           |

- All the results are in agreement!
- Problem when $Q$ is large!
- Comparison with the other method (still a bit early)
  - Seems to give similar results.
  - The implementation of the second method is a bit less costly but both are cheap.
  - Works also for large volume!
Systematic errors due to topology freezing!
No straightforward way of calculating the topological susceptibility at fixed topology!

Two simple methods to extract topological susceptibility:

- **AFHO method**: precise results, but not suitable for large volume.
- **Slab method**: precise results, suitable for large volume.

We have still some works:

- A deeper analysis of the effects of gradient flow on both methods to extract topological susceptibility has to be done.
- Analyze the influence of the subvolume shape in the slab method.