The QCD topological susceptibility at finite temperature: a new investigation with staggered spectral projectors

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LATTICE GAUGE THEORY CONTRIBUTIONS TO NEW PHYSICS SEARCHES 12–16/06/2023, Madrid

#### Based on:

"Topological susceptibility of  $N_f = 2 + 1$  QCD from staggered fermions spectral projectors at high temperatures",

A. Athenodorou, CB, C. Bonati, G. Clemente, F. D'Angelo, M. D'Elia, L. Maio, G. Martinelli, F. Sanfilippo, A. Todaro, JHEP 10 (2022) 197 [2208.08921]

## Non-chiral fermions and would-be-zero modes

Lattice QCD is a natural non-perturbative tool to compute  $\chi(T)$  from first-principle. However: several non-trivial computational challenges.

In the QCD path-integral, field configurations are weighted with the determinant of the Dirac operator:

$$\langle \mathcal{O} \rangle = \frac{\int [dA] e^{-S_{\rm YM}[A]} \prod_f \det\{ \not\!\!D[A] + m_f \} \mathcal{O}[A]}{\int [dA] e^{-S_{\rm YM}[A]} \prod_f \det\{ \not\!\!D[A] + m_f \}}, \qquad \det\{ \not\!\!D + m_f \} = \prod_{\lambda \in \mathbb{R}} \left( i\lambda + m_f \right).$$

In the continuum, Dirac determinant suppresses contribution of non-zero Q configurations to  $\langle \mathcal{O} \rangle$  as a power of the quark mass (because of index theorem):

$$Q[A] = n_0^{(L)} - n_0^{(R)} \implies \det\{\mathcal{D}[A] + m_f\} \propto m_f^{\alpha}$$

Typical lattice fermionic discretizations (e.g., Wilson, staggered) do not have exact zero-modes due to explicit breaking of chiral symmetry at finite lattice spacing → No exact zero-mode appears in the spectrum, and determinant fails to efficiently suppress non-zero charge configurations

 $\lambda_{\min} = m_f \longrightarrow m_f + i\lambda_{\text{would-be-zero}}$ 

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## Would-be-zero modes and large lattice artifacts

Bad suppression of non-zero charge configurations due to would-be-zero modes  $\implies$  large lattice artifacts affect the standard gluonic computation of  $\chi$  $\Rightarrow$  continuum extrapolation not under control (Bonati et al., 2018 [1807.07954])



Strategy followed in (Borsanyi et al., 2016 [1606.07494]) to reduce lattice artifacts affecting  $\chi$  at high-T: reweighting configurations a posteriori with corresponding continuum lowest eigenvalues of D.

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## Fermionic topological charge

Different possible solution, which does not require further assumptions: switch, through the Index Theorem, to fermionic definitions of Q. Using the same "bad" operator to weight configurations and to count eigenmodes to measure Q may introduce smaller lattice artifacts.



Idea supported by results at T = 0 (Alexandrou et al., 2017 [1709.06596]): Twisted Mass (TM) Wilson fermions employed for the Monte Carlo evolution and to measure  $\chi$  through spectral projectors on eigenmodes of  $D_{\rm TM} \longrightarrow$  improved scaling of  $\chi$  towards the continuum!

Main results of our work [2208.08921]: use staggered fermions spectral projectors definition (CB et al., 2019 [1908.11832]) to reduce lattice artifacts and study  $\chi(T)$  at high T from

full QCD simulations with staggered fermions.

## Spectral projectors with staggered fermions

In the continuum, only zero-modes contribute to Q. On the lattice, spectral sum are extended up to a certain cut-off M:

$$Q = \sum_{\lambda = 0} u_{\lambda}^{\dagger} \gamma_5 u_{\lambda} \longrightarrow \sum_{|\lambda| \le M} u_{\lambda}^{\dagger} \Gamma_5 u_{\lambda} = \operatorname{Tr} \{ \Gamma_5 \mathbb{P}_M \},$$
$$\mathbb{P}_M = \sum_{|\lambda| \le M} u_{\lambda} u_{\lambda}^{\dagger}, \qquad i D_{\operatorname{stag}} u_{\lambda} = \lambda u_{\lambda}, \quad \lambda \in \mathbb{R}.$$

$$Q_{0,\mathrm{SP}} = \frac{1}{n_t} \sum_{|\lambda| \leq M} u_\lambda^\dagger \Gamma_5 u_\lambda$$

Taste degeneration leads to mode over-counting  $\implies$  divide spectral sum by the number of tastes  $(n_t = 4)$ 

Lattice charge gets mult. renormalization  $Z_Q^{(\text{stag})} = Z_P/Z_S$ , which can be derived from Ward identities for the flavor-singlet axial current:

$$Q_{\rm SP} = \frac{Z_P}{Z_S} Q_{0,\rm SP}, \qquad \left(\frac{Z_P}{Z_S}\right)^2 = \frac{\langle \operatorname{Tr}\{\mathbb{P}_M\}\rangle}{\langle \operatorname{Tr}\{\Gamma_5 \mathbb{P}_M \Gamma_5 \mathbb{P}_M\}\rangle},$$
$$\chi_{\rm SP} = \langle Q_{\rm SP}^2 \rangle / V.$$

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## Choice of the cut-off mass M

The choice of the cut-off mass M is irrelevant in the continuum limit. Its renormalized value  $M_R = M/Z_S$  must be kept constant as  $a \to 0$  to guarantee  $O(a^2)$  corrections:

$$\chi_{\rm SP}(a, M_R) = \chi + c_{\rm SP}(M_R)a^2 + o(a^2).$$

To avoid the direct computation of  $Z_S$  for each lattice spacing, one can observe that, for staggered fermions:

$$m_q^{(R)} = m_q / Z_S.$$

If a Line of Constant Physics (LCP) is known, it is sufficient to keep

$$M/m_q = M_R/m_q^{(R)}$$

constant along the LCP as  $a \to 0$  to keep  $M_R$  constant.

How do we choose  $M_R$ ? One would like to have small corrections, i.e.,  $c_{\rm SP}(M_R) \ll c_{\rm gluo}.$ 

## Rare topological fluctuations and multicanonic algorithm

Since  $\chi$  is suppressed at high T, on affordable volumes:  $\langle Q^2 \rangle = \chi V \ll 1$ 

 $\implies Q$  fluctuations extremely rare during Monte Carlo evolution.

Adopted solution: multicanonic algorithm.

$$S_{\text{QCD}}^{(L)} \to S_{\text{QCD}}^{(L)} + V_{\text{topo}}(Q_{\text{mc}})$$
  
$$\implies P \propto e^{-S_{\text{QCD}}^{(L)}} \to P_{\text{mc}} \propto e^{-S_{\text{QCD}}^{(L)}} e^{-V_{\text{topo}}(Q_{\text{mc}})}$$

Idea: add bias potential to the action to enhance the probability of visiting suppressed topological sectors.

Mean values  $\langle \rangle$  with respect to P recovered through reweighting:



Choice of the cut-off mass  $M/m_s$  (finite T)

Determine range for  $M/m_s$  from scatter plot of chirality  $r_{\lambda} = |u_{\lambda}^{\dagger}\Gamma_5 u_{\lambda}|$  vs  $|\lambda|/m_s$ .

Finite T: more clear separation among WBZMs and non-chiral modes  $\longrightarrow$  however, completely unambiguous separation not possible



Fig:  $N_f = 2 + 1, V = 48^3 \times 16$ 

Vertical lines  $\rightarrow$  range in which  $M/m_s$  is varied:  $M/m_s \in [0.3, 5].$ 

# Continuum limit of $\chi^{1/4}$ at finite T (T = 430 MeV)

Lattice setup: tree-level Symanzik-improved gauge action + 2 + 1 flavors of rooted stout staggered fermions at the physical point. Continuum-scaling:

$$\begin{split} \chi^{1/4}_{\rm SP}(a,M/m_s) &= \chi^{1/4} + c_{\rm SP}(M/m_s)a^2 + o(a^2). \\ \chi^{1/4}_{\rm gluo}(a) &= \chi^{1/4} + c_{\rm gluo}a^2 + o(a^2). \end{split}$$



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## Continuum extrapolation T = 430 vs $M/m_s$

Choosing  $M/m_s$  inside the determined range we observe:

- good agreement within the errors for determinations obtained for different values of  $M/m_s$  (Fig. on the left)
- significant reduction of lattice artifacts compared to the standard gluonic computation can be achieved with suitable choice of  $M/m_s$  (Fig. on the right)



## $\chi(T)$ for $T > T_c$ from staggered Spectral Projectors

We computed  $\chi(T)$  for 200 MeV  $\lesssim T \lesssim 600$  MeV. Comparison with Dilute Instanton Gas Approximation (DIGA):

DIGA:  $\chi^{1/4}(T) \sim (T/T_c)^{-b}, \quad b \simeq 2 \text{ (3 flavors)}.$ 



Data for  $T \gtrsim 300$  MeV: very good agreement with **DIGA-like power law**:

$$b_{\rm SP} = 2.1(4), \qquad b_{\rm gluo} = 2.3(1.1)$$

If we also include also point for T = 230 MeV (lowest T explored):

$$b_{\rm SP} = 1.8(4), \qquad b_{\rm gluo} = 1.7(5)$$

Results compatible within errors, but slope clearly changes if T = 230 MeV is included/excluded.

Could be a (not conclusive) indication of a change in eff. exp. b between 200 and 300 MeV.

Clear consensus among different lattice determinations of  $\chi(T)$  still to be reached  $\longrightarrow$  would be interesting to further inquire the region  $T \lesssim 400$  MeV

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#### BACKUP SLIDES

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## Choice of the cut-off mass M (T = 0 example)

**Guiding principle**: choose  $M/m_s$  to include all relevant Would-Be Zero-Modes (WBZMs) in spectral sums. E.g., look at chirality:  $r_{\lambda} = |u_{\lambda}^{\perp} \Gamma_5 u_{\lambda}|$  vs  $|\lambda|/m_s$ .

However, distinguishing between WBZMs and non-chiral modes is ambiguous  $\rightarrow$ 

- Choose a range of cut-offs to include "chiral enough" modes
- Perform continuum extrapolation for several values of  $M/m_s$  and check its stability



Fig:  $N_f = 2 + 1, V = 48^4$ .

Vertical lines  $\rightarrow$  range in which  $M/m_s$  is varied:  $M/m_s \in [0.05, 0.15]$ 

## Continuum limit of $\chi^{1/4}$ at T = 0

0.75

 $a^2 \, [fm^2]$ 

 $\chi^{1/4}$  [MeV]

0.25

0.50

0.00

Lattice Setup:  $N_f = 2 + 1$  rooted stout staggered fermions at physical point. Expected continuum scaling for Spectral Projectors (SP):

 $\gamma_{ap}^{1/4}(a, M/m_{a}) = \gamma^{1/4} + c_{sp}(M/m_{a})a^{2} + o(a^{2}).$ 

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 $1.50 \\ \times 10^{-2}$ 

1.25

1.00

## Continuum extrapolation at T = 0 vs $M/m_s$

Choosing  $M/m_s$  inside the determined range we observe:

- $\bullet\,$  good agreement within the errors for determinations obtained for different values of  $M/m_s$  (Fig. on the left)
- significant reduction of lattice artifacts compared to the standard gluonic computation (Fig. on the right)



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