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

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EXCELENCIA SEVERO OCHOA

New Trends in Thermal Phases of QCD
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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]

Motivations

- *Topology and the Dirac spectrum*

Index theorem relates gauge topology with low-lying Dirac spectrum

$$Q = \frac{1}{16\pi^2}\int d^4x \, \mathrm{Tr}\left\{G_{\mu\nu}(x)\widetilde{G}^{\mu\nu}(x)\right\} \in \mathbb{Z}, \qquad Q = n_0^{(L)} - n_0^{(R)}.$$

Intruiguing interplay between gauge topology and chiral properties of fermions.

Studying thermodynamics of QCD topology
$\longrightarrow$ deeper insight into the non-perturbative properties of the theory.

- *Strong*-CP *violation and axion phenomenology*

QCD admits CP-violation via the θ-term, coupling Q to S_{QCD}.
The QCD axion, introduced to dynamically relax θ to 0, has been considered as a Dark Matter candidate.
The behavior of the axion effective parameters at high temperatures is extremely relevant for cosmology $\longrightarrow$ essential input for present and future experimental searches.

$$\chi(T) \equiv \lim_{V\to\infty} \frac{\langle Q^2\rangle_T}{V} \propto m_a^2(T)$$

Axion phenomenology requires QCD inputs for the T-dependence of χ in the high-temperature regime.

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:

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

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):

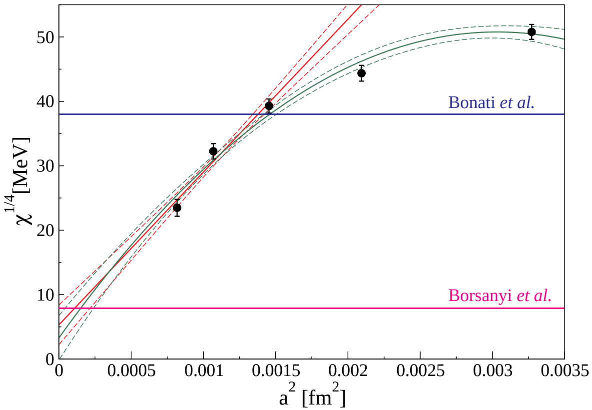
$$Q[A] = n_0^{(L)} - n_0^{(R)} \implies \det\{\not{D}[A] + m_f\} \propto m_f^{\alpha}$$

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
$\implies$ No exact zero-mode appears in the spectrum, and determinant fails to efficiently suppress non-zero charge configurations

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

Would-be-zero modes and large lattice artifacts

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

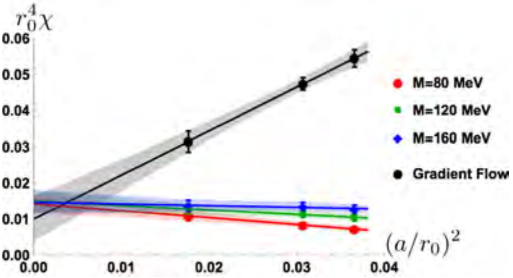


Strategy followed in (Borsanyi et al., 2016 [1606.07494]) to reduce lattice artifacts affecting χ at high-T: reweighting configurations a posteriori with corresponding continuum lowest eigenvalues of $\not{D}$.

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 χ through spectral projectors on eigenmodes of $D_{\mathrm{TM}} \longrightarrow$ improved scaling of χ 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:

$$Q = \sum_{\lambda=0} u_\lambda^\dagger \gamma_5 u_\lambda \longrightarrow \sum_{|\lambda|\leq M} u_\lambda^\dagger \Gamma_5 u_\lambda = \mathrm{Tr}\{\Gamma_5 \mathbb{P}_M\},$$

$$\mathbb{P}_M = \textstyle\sum_{|\lambda|\leq M} u_\lambda u_\lambda^\dagger, \qquad iD_{\mathrm{stag}} u_\lambda = \lambda u_\lambda, \quad \lambda \in \mathbb{R}.$$

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

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

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

$$Q_{\mathrm{SP}} = \frac{Z_P}{Z_S} Q_{0,\mathrm{SP}}, \qquad \left(\frac{Z_P}{Z_S}\right)^2 = \frac{\langle \mathrm{Tr}\{\mathbb{P}_M\}\rangle}{\langle \mathrm{Tr}\{\Gamma_5 \mathbb{P}_M \Gamma_5 \mathbb{P}_M\}\rangle},$$

$$\chi_{\mathrm{SP}} = \langle Q_{\mathrm{SP}}^2 \rangle / V.$$

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:

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

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., $c_{\mathrm{SP}}(M_R) \ll c_{\mathrm{gluo}}$.

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: $r_\lambda = |u_\lambda^\dagger \Gamma_5 u_\lambda|$ vs $|\lambda|/m_s$.

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

- 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

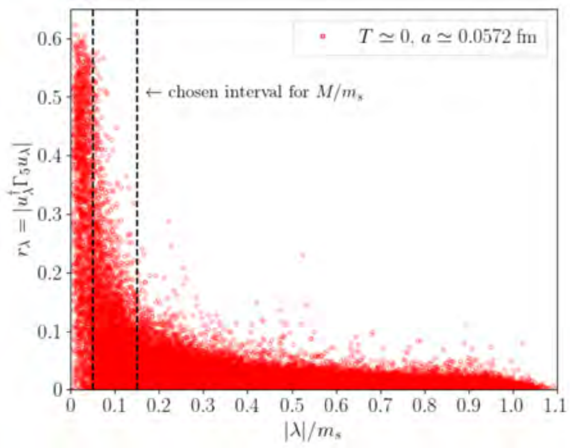


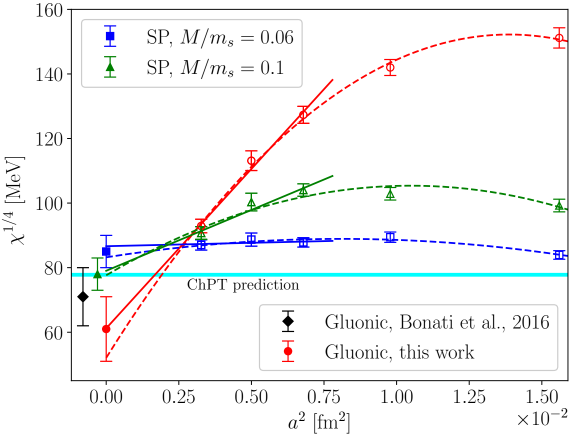
Fig: $N_f = 2+1$, $V = 48^4$.

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 $T = 0$

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

$$\chi_{\rm SP}^{1/4}(a, M/m_s) = \chi^{1/4} + c_{\rm SP}(M/m_s)a^2 + o(a^2).$$



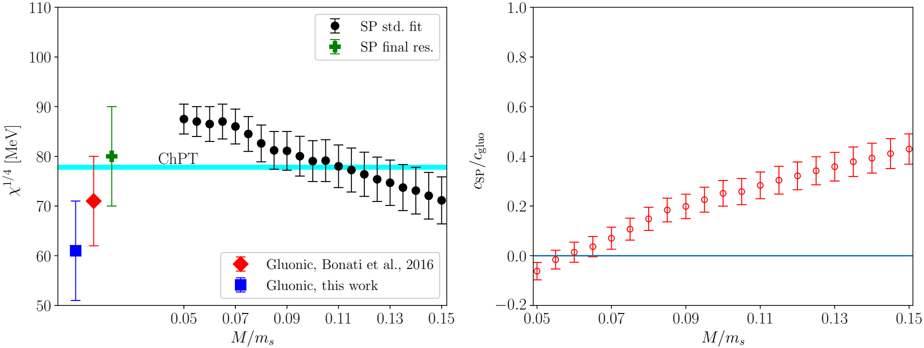
M/m_s inside determined interval $\rightarrow$ reduction of lattice artifacts:
$c_{\rm SP}(0.06)/c_{\rm gluo} \sim 1 \cdot 10^{-2}$,
$c_{\rm SP}(0.1)/c_{\rm gluo} \sim 3 \cdot 10^{-1}$.

Spectral determination: very good agreement with gluonic and NLO Chiral Perturbation Theory (ChPT) prediction.

Continuum extrapolation at $T = 0$ 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 (Fig. on the right)



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

Same strategy as $T = 0$: 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

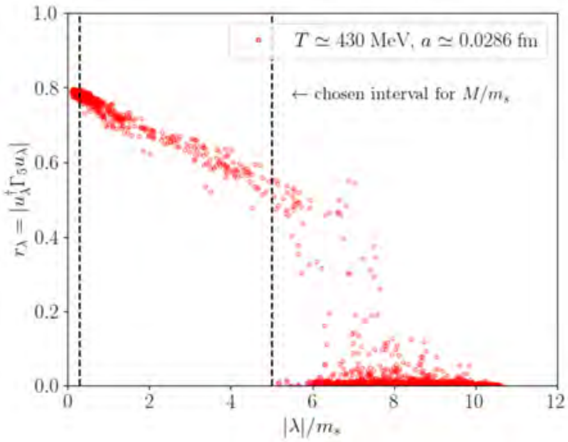


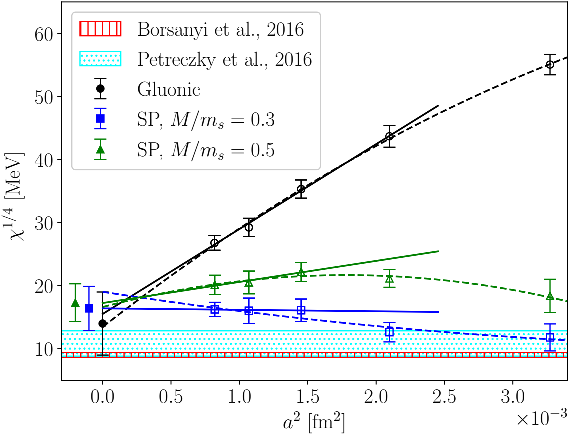
Fig: $N_f = 2 + 1$, $V = 48^3 \times 16$

Vertical lines $\to$ 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)

Same lattice setup of $T = 0$ case. Also, same continuum-scaling function for Spectral Projectors (SP):

$$\chi_{\mathrm{SP}}^{1/4}(a, M/m_s) = \chi^{1/4} + c_{\mathrm{SP}}(M/m_s)a^2 + o(a^2).$$



Spectral lattice artifacts are suppressed compared to the gluonic case when M/m_s is chosen within the determined interval:

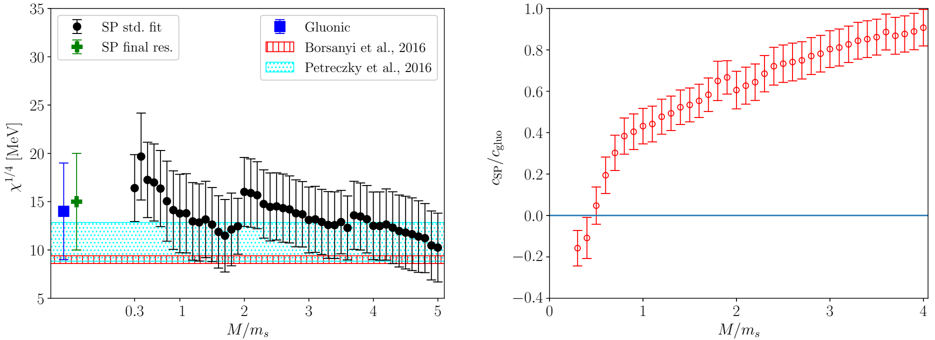
$c_{\mathrm{SP}}(0.3)/c_{\mathrm{gluo}} \sim 5 \cdot 10^{-2}$,

$c_{\mathrm{SP}}(0.5)/c_{\mathrm{gluo}} \sim 10^{-1}$.

Continuum extrapolation $T = 430$ vs M/m_s

Choosing M/m_s inside the determined range we observe:

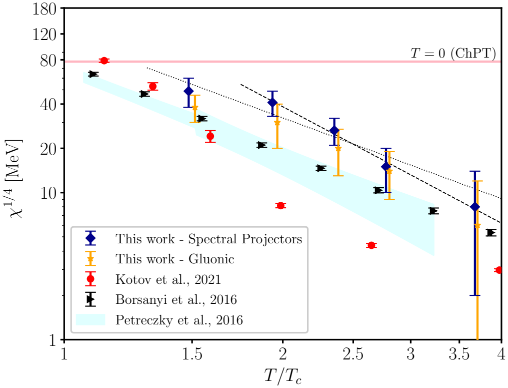
- good agreement within the errors for determinations obtained for different values of M/m_s (Fig. on the left)
- significant reduction of lattice artifacts compared to the standard gluonic computation can be achieved with suitable choice of M/m_s (Fig. on the right)



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



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

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

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

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

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

Further studies of the $T \lesssim 300$ MeV regime

Our results for $\chi(T)$ fit well with recent observations suggesting that high-T QCD is dominated by non-perturbative effects for $T_c \lesssim T \lesssim 300$ MeV (Alexandru & Horváth, 2019 [1906.08047], 2021 [2103.05607]; Kotov et al., 2021 [2105.09842]; Cardinali et al. 2021 [2107.02745])

Further investigation: computation of staggered **spectral density** on our full QCD ensembles at $T = 230$ MeV. Also motivated by results of [1906.08047]: $200 \text{ MeV} < T_{\text{IR}} < 250 \text{ MeV}$

(work in progress in collaboration with A. Alexandru, M. D'Elia & I. Horváth)

$$\rho(\lambda) = \frac{\langle \# \lambda \in \text{Bin} \rangle}{n_t V \Delta\lambda}, \qquad \text{Bin} = \left[\lambda - \frac{\Delta\lambda}{2}, \lambda + \frac{\Delta\lambda}{2} \right].$$

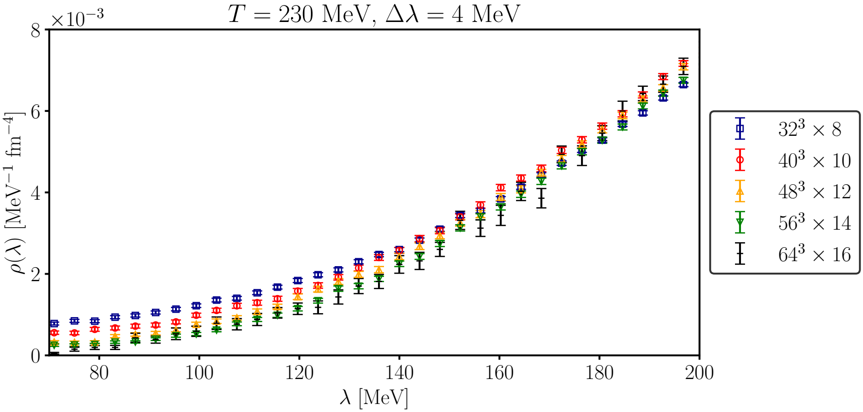
An eigenvalue λ of iD_{stag} renormalizes as m_q $\rightarrow$ use same $\Delta\lambda / m_s$ for each ensemble, with m_s drawn from LCP at physical point:

$$m_s \rho(\lambda / m_s) = \frac{\langle \# \lambda / m_s \in \text{Bin} / m_s \rangle}{n_t V (\Delta\lambda / m_s)}$$

is expected to be a properly renormalized physical quantity.

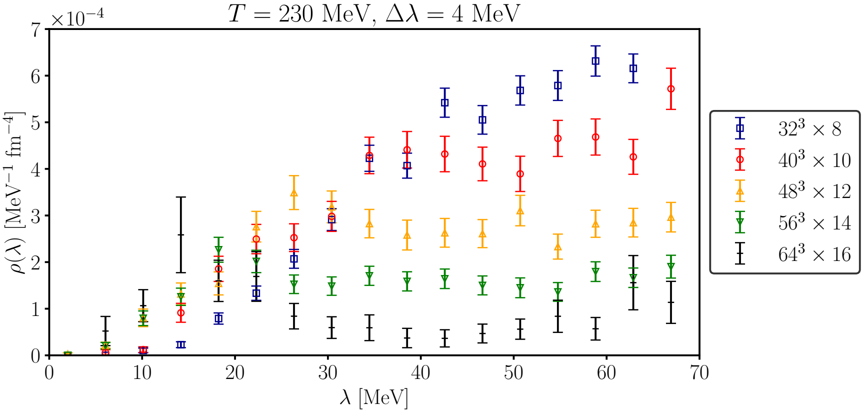
Staggered spectral density in full QCD - 1

- Same spatial volume $V_s \simeq (3.4 \text{ fm})^3$
- Lattice spacing ranging from ~ 0.1 fm to ~ 0.054 fm
- $m_s^{(\text{FLAG21})} = 92.2(1.0)$ MeV [2111.09849] used to express $\Delta\lambda$ and $V\rho(\lambda)$ in phys. units



Spectral density is found to be a monotonically rising function in the region above ~ 80 MeV. Lattice artifacts appear more pronounced below ~ 150 MeV.

Staggered spectral density in full QCD - 2



- Between ~ 20 and ~ 70 MeV, $\rho(\lambda)$ is almost constant, and its value decreases as we approach the continuum limit
- Below ~ 20 MeV lattice artifacts go in the opposite direction, and $\rho(\lambda)$ grows as a is reduced
- These features fit well with results of [1906.08047] and [2103.05607] obtained for the IR phase with D_{overlap}, and also with well-established results on localitazion/delocalization transition in the Dirac spectrum (Giordano & Kovacs, 2021 [2104.14388])

Conclusions

Summary of the talk:

- Spectral Projectors (SP) provide a theoretically well-posed method to define the topological susceptibility on the lattice
- Spectral definition of χ allows to control the magnitude of lattice artifacts through a smart choice of the cut-off mass M also at non-zero temperature
- SP results are well described by DIGA law $\chi^{1/4}(T) \sim (T/T_c)^{-2}$ for $T \gtrsim 300$ MeV
- Possible deviations from DIGA-like scaling possibly related to strong non-perturbative effects in the $T \lesssim 300$ MeV regime $\longrightarrow$ deserves further studies

Future outlooks

- computing χ for $T \gtrsim 700$ MeV on typical lattices requires $a \sim 0.01$ fm $\implies$ severe Topological Slowing Down. Promising candidate algorithm: **Parallel Tempering on Boundary Conditions** (Hasenbusch, 2017 [1706.04443]; CB et al., 2021 [2012.14000])
- Further studies of the spectral density for $T = 230$ MeV (larger volume, continuum limit, staggered vs overlap spectral density comparison ...)

Rare topological fluctuations and multicanonic algorithm

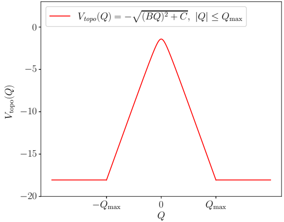
Since χ is suppressed at high T, on affordable volumes: $\langle Q^2 \rangle = \chi V \ll 1$
$\Longrightarrow$ Q fluctuations extremely rare during Monte Carlo evolution.
Adopted solution: multicanonic algorithm.

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

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:

$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} e^{V_{\mathrm{topo}}(Q_{\mathrm{mc}})} \rangle_{\mathrm{mc}}}{\langle e^{V_{\mathrm{topo}}(Q_{\mathrm{mc}})} \rangle_{\mathrm{mc}}}, \qquad \langle \mathcal{O} \rangle_{\mathrm{mc}} \to \text{ mean value with respect to } P_{\mathrm{mc}}$$



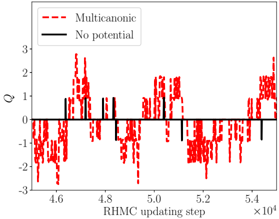


Fig: $32^3 \times 8$ lattice,
$T = 430$ MeV,
$a \simeq 0.057$ fm.

$Q_{\mathrm{mc}} \to$ clover charge computed on stout-smeared fields after $n_{\mathrm{stout}} = 10$ steps.