The Peccei–Quinn axion and QCD topology

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NEUTRON ELECTRIC DIPOLE MOMENT: FROM THEORY TO EXPERIMENT

01–05/08/2022 - ECT*, Trento

The strong-CP problem

QCD admits CP-violations by the topological term

$$S_{\rm QCD} = S_{\rm YM} + S_{\rm ferm} \to S_{\rm QCD}(\theta) = S_{\rm QCD} + \theta Q$$

$$Q = \frac{1}{16\pi^2}\int {\rm Tr}\left[G_{\mu\nu}(x)\widetilde{G}^{\mu\nu}(x)\right]\, d^4x \in \mathbb{Z}$$

Experimental measure of the neutron Electric Dipole Moment (nEDM) $|\vec{d}_N|$ puts the most stringent upper bound:

- $|\vec{d}_N| = |0.9 \pm 2.4| \cdot 10^{-3}\ |\theta|\ e \cdot {\rm fm}$ (Lattice QCD – Alexandrou et al., 2020)
- $|\vec{d}_N| = (2.9 \pm 0.9) \cdot 10^{-3}\ |\theta|\ e \cdot {\rm fm}$ (ChPT – Guo, Meißner, 2012)
- $|\vec{d}_N| \lesssim 1.8 \cdot 10^{-13}\ e \cdot {\rm fm}$ (PSI measure – Abel et al., 2020)

$\Longrightarrow$ θ is either vanishing or unnaturally small: $|\theta| \lesssim 10^{-10}$.

Problem: $\theta = 0$ is special because CP $Q = -Q$

$\Longrightarrow$ $S_{\rm QCD}(\theta)$ is invariant under CP only if $\theta = 0$ ($\theta = \pi \to$ SSB)

$\longrightarrow$ fine tuning issue known as strong-CP problem.

Possible solutions to the strong-CP problem

Several dynamical solutions to strong-CP problem have been proposed:

- If up quark has $m_u = 0$, under $\mathrm{U}(1)_\mathrm{A}$ S_QCD gets just an anomalous variation:

$$\begin{aligned} u &\to e^{i\gamma_5\alpha}u \\ S_\mathrm{QCD}(\theta) &\to S_\mathrm{QCD}(\theta) - 2\alpha Q = S_\mathrm{QCD}(\theta - 2\alpha) \end{aligned}$$

  Choosing $2\alpha = \theta \to S_\mathrm{QCD}(\theta) = S_\mathrm{QCD}(\theta = 0)$. **Ruled out by lattice results:** $m_u = 2.14(8)$ **MeV (FLAG Review 2021)**.

- Other dynamical solutions within QCD have been proposed (see, e.g., talks by B. Garbrecht, G. Schierholz and C. Tamarit in this workshop).

- Beyond Standard Model (SM) solutions such as the Peccei–Quinn axion.

The Peccei–Quinn axion

The axion solution (Peccei, Quinn, 1977; Weinberg, 1978; Wilczek, 1978) requires to supplement SM with few new ingredients:

- new global axial abelian symmetry $\mathrm{U}(1)_{\mathrm{PQ}}$,
- $\mathrm{U}(1)_{\mathrm{PQ}}$ is spontaneously broken at $\sim f_a$,
- axion scale extremely large: 10^8 GeV $\lesssim f_a \lesssim 10^{12}$ GeV.

This simple recipe provides dynamical mechanism (PQ mechanism) to solve the strong-CP problem:

- new light pseudo Nambu-Goldstone boson: the PQ axion;
- by anomaly matching the term $\left(\frac{a}{f_a} - \theta\right) q(x)$ is effectively generated at scales $\ll f_a$ (indep. of UV completions; see, e.g., talk by L. Covi);
- axion shift symmetry $a \underset{\mathrm{U}(1)_{\mathrm{PQ}}}{\to} a - \alpha f_a$ relaxes $\theta = 0$ choosing $\alpha = \theta$.

Bonus: axion couplings to SM particles are suppressed as $f_a \implies$ axion is a possible Dark Matter candidate and may play an important cosmological role.

Axion cosmology

Evolution of the axion field a in the FLRW metric:

$$\ddot{a} + 3H\dot{a} + \frac{dV_{\text{eff}}(a)}{da} = 0, \qquad V_{\text{eff}}(a) = \frac{1}{2}m_a^2 a^2 + \ldots, \qquad H \equiv \frac{\dot{R}}{R} = \text{ Hubble rate}$$

Define the temperature T_{osc} as $3H(T_{\text{osc}}) \equiv m_a(T_{\text{osc}})$:

- $T \gg T_{\text{osc}}$: friction term $3H$ dominates over mass term $m_a \to \theta = \theta_0 \neq 0$,
- $T \sim T_{\text{osc}}$: axion starts to feel the potential and descends towards the minimum (corresponding to $\theta = 0$) $\to$ axion production;
- $T \ll T_{\text{osc}}$: mass term dominates over friction term $\to$ decaying oscillations around the minimum $\to$ $\theta = 0$ & axion number freezes.

Solving Einstein + axion equations gives Ω_a (axion energy density), which can account for (part of) the observed Dark Matter (DM) energy density.

Once $V_{\text{eff}}(a)$ (most importantly, the mass m_a) is plugged into the game, this procedure gives Ω_a as a function of f_a. Comparing Ω_a with the experimentally observed Ω_{DM}, one can put a theoretical bound on the axion scale f_a.

Axion physics and θ-dependence in QCD

The θ-dependent QCD free energy (density) can be expressed in terms of the Euclidean path integral:

$$f_{\mathrm{QCD}}(\theta) = -\frac{1}{V} \log \int [dA] e^{-S_{\mathrm{YM}} + i\theta Q} \prod_{f=1}^{N_f} \det \left\{ \not{D} + m_f \right\}.$$

By virtue of the interaction term proportional to the charge density:

$$\mathcal{L}_{\mathrm{QCD}}(\theta) + \mathcal{L}_a = \mathcal{L}_{\mathrm{QCD}} + \frac{1}{2}\partial_\mu a \partial_\mu a + i\left(\frac{a}{f_a} - \theta\right) q(x), \quad Q = \int q(x)\, d^4x,$$

the following relation holds (integrating out QCD sector):

$$V_{\mathrm{eff}}(a) = f_{\mathrm{QCD}}\left(\theta = \frac{a}{f_a}\right).$$

It is thus clear that theoretical predictions regarding axion cosmology need the **QCD input** about the θ-dependence of the QCD free energy.

Axion field cosmological evolution

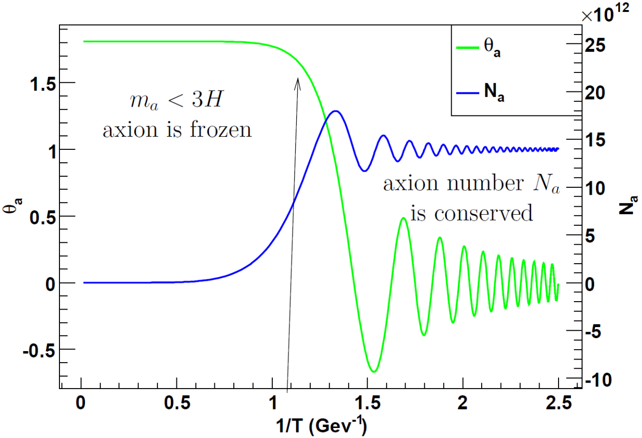


Figure adapted from "*Axion Cosmology Revisited*", O. Wantz and E.P.S. Shellard, Phys. Rev. D **82** (2010) 123508 [arXiv:0910.1066]

θ-dependence of the free energy in QCD

The θ-dependent QCD free energy

$$f_{\mathrm{QCD}}(\theta) = -\frac{1}{V}\log\int[dA]e^{-S_{\mathrm{YM}}+i\theta Q}\prod_{f=1}^{N_f}\det\left\{\not{D}+m_f\right\}$$

is an even function of θ that is usually parametrized as

$$f_{\mathrm{QCD}}(\theta) - f_{\mathrm{QCD}}(0) = \frac{1}{2}\,\chi\theta^2\left(1+b_2\theta^2+b_4\theta^4+\ldots\right),$$

$$V_{\mathrm{eff}}(a) = \frac{1}{2}\,m_a^2a^2\left(1+\lambda_2a^2+\lambda_4a^4+\ldots\right).$$

The coefficients are related to the **cumulants** of the topological charge distribution at $\theta=0$. For example:

$$\chi = \left.\frac{\langle Q^2\rangle}{V}\right|_{\theta=0} = \frac{m_a^2}{f_a^2} \qquad \textbf{(Topological Susceptibility)}$$

$$b_2 = -\frac{1}{12}\left.\frac{\langle Q^4\rangle-3\langle Q^2\rangle^2}{\langle Q^2\rangle}\right|_{\theta=0} \qquad \text{(First non-quadratic correction)}$$

QCD θ-dependence at $T = 0$: Chiral Perturbation Theory

Effective theory with pseudo Nambu–Goldstone bosons (**pions**) as dof:

$$\mathcal{L}_{\rm eff}^{(\rm LO)}(U) = \frac{f_\pi^2}{4}\partial_\mu U \partial^\mu U^\dagger + \frac{\Sigma}{4}\Re\left\{U M_q^\dagger\right\}, \qquad U = e^{i\frac{\pi_a}{f_\pi}\tau_a},\ \Sigma = -\langle\overline{\psi}\psi\rangle$$

How to study θ dependence? Trade θ-term for a **phase** in quark mass matrix:

$\psi \to e^{i\gamma_5\alpha}\psi$	$\mathrm{U(1)_A}$ transformation
$\overline{\psi}_L M_q \psi_R \to e^{2i\alpha}\overline{\psi}_L M_q \psi_R$	non invariance of mass term
$\theta \to \theta - 2\alpha N_f$	anomaly

Choosing $\alpha = \theta/(2N_f)$, θ is fully moved into quark mass matrix M_q:

$$\mathcal{L}_{\rm eff}^{(\rm LO)}(U,\theta) = \tfrac{f_\pi^2}{4}\partial_\mu U \partial^\mu U^\dagger + \tfrac{\Sigma}{4}\Re\left\{e^{i\theta/N_f} U M_q^\dagger\right\}.$$

Free energy is obtained from field configuration $U_{\rm min}(\theta)$ minimizing $\mathcal{L}_{\rm eff}^{(\rm LO)}(U,\theta)$:

$$f_{\rm ChPT}^{(\rm LO)}(\theta) = \frac{1}{V}\mathcal{L}_{\rm eff}^{(\rm LO)}\left(U_{\rm min}(\theta),\theta\right)$$

$$(N_f = 2) \qquad f_{\rm ChPT}^{(\rm LO)}(\theta) = m_\pi^2 f_\pi^2 \sqrt{1 - \frac{4 m_u m_d}{(m_u + m_d)^2}\sin^2\left(\frac{\theta}{2}\right)}$$

Main ChPT results about θ-dependence

At LO with (u, d) quarks, topological quantities can be expressed in terms of f_π, m_π and $z = m_u/m_d$ (Di Vecchia and Veneziano, 1980; Leutwyler and Smilga, 1992):

$$\chi_{\mathrm{LO-ChPT}} = \frac{z}{(1+z)^2} m_\pi^2 f_\pi^2, \qquad b_2^{(\mathrm{LO-ChPT})} = -\frac{1}{12}\frac{1+z^3}{(1+z)^3}.$$

Also NLO corrections are known for χ and b_2 (Di Cortona, 2016)

$$\chi_{\mathrm{NLO-ChPT}} = (77.8(4)\ \mathrm{MeV})^4, \qquad m_u = m_d$$

$$\chi_{\mathrm{NLO-ChPT}} = (75.5(5)\ \mathrm{MeV})^4, \qquad \text{physical } m_u, m_d$$

For comparison, result for the quenched theory (see also M. D'Elia's talk):

$\chi_{\mathrm{YM}} \simeq (180\ \mathrm{MeV})^4$, (Witten–Veneziano Eq.; Bonati et al., 2016; CB et al., 2021)

$$b_2^{\mathrm{NLO-ChPT}} = -0.029(2), \qquad m_u = m_d$$

$$b_2^{\mathrm{NLO-ChPT}} = -0.022(1), \qquad \text{physical } m_u, m_d$$

$$b_2^{(\mathrm{YM})} \simeq -0.0216(5),$$ (Bonati et al., 2016, CB et al., 2021)

Results so far: $T = 0$. ChPT provides also finite-T results which are expect to hold below T_c.

QCD θ-dependence at high T: Dilute Instanton Gas Approximation (DIGA)

For $T > T_c$, ChPT breaks down. For asymptotically-large $T \gg \Lambda_{\mathrm{QCD}}$: semi-classical approximation + perturbation theory → **Dilute Instanton Gas Approximation** (DIGA) (Gross, Pisarski, Yaffe, 1981; Schäfer & Shuryak, 1998; Boccaletti & Nogradi, 2020)

$$f_{\mathrm{DIGA}}(T,\theta) = \left(\frac{2Z_1(T)}{V}\right)(1-\cos\theta) \equiv \chi(T)\,(1-\cos\theta)$$

From diluteness assumption

$$\chi\,(1-\cos\theta) \leftrightarrow \frac{\chi\theta^2}{2}\left(1+b_2\theta^2+\dots\right) \implies b_2^{(\mathrm{DIGA})} = -\frac{1}{12} \simeq -0.083$$

$$\chi(T) \underset{T\gg\Lambda_{\mathrm{QCD}}}{\sim} T^{-c}$$

Perturbation around 1 instanton

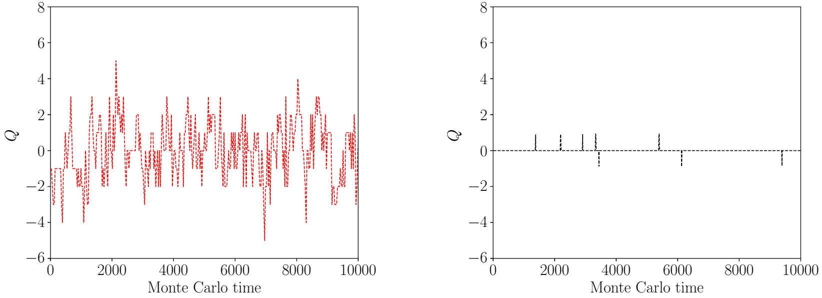
$$c = 4 - \frac{1}{3}N_f - \frac{11}{3}N_c$$

($c = 8$ for 3 light flavors)

Axion cosmology interesting range: $T \gg T_c$ down to $\sim$ GeV scale
$\implies$ **non-perturbative** physics dominate when T close to QCD scale
Non-perturbative lattice QCD needed to fully control $\chi(T)$ above T_c

At high T χ is suppressed, thus $\langle Q^2 \rangle = V\chi \ll 1$. The probability of visiting $|Q| \neq 0$ sectors is **strongly suppressed** at high-T on typical lattice volumes.

An example for the same lattice spacing $a \simeq 0.0572$ fm



(a) 48^4 lattice, $T \simeq 0$ (b) $32^3 \times 8$ lattice, $T \simeq 430$ MeV

If $P_0 \equiv P(Q = 0) \gg P_1 \equiv P(|Q| = 1) \gg P(|Q| = 2)$, we have:

$$\chi = \frac{1}{V} \langle Q^2 \rangle = \frac{1}{V} \frac{0^2 P_0 + 2P_1 + \dots}{P_0 + P_1 + \dots} \simeq \frac{2}{V} \frac{P_1}{P_0}$$

Topology, chiral symmetry and Dirac zero-modes

Configurations are weighted in the path integral according to the fermion determinant

$$e^{-V f_{\mathrm{QCD}}(\theta)} = \int [dA] e^{-S_{\mathrm{YM}} + i\theta Q} \prod_{f=1}^{N_f} \det\left\{ \not{D} + m_f \right\}$$

$$\det\{\not{D} + m_f\} = \prod_{\lambda \in \mathbb{R}} (i\lambda + m_f) = m_f^{n_0} \prod_{\lambda > 0} (\lambda^2 + m_f^2)\,.$$

The *Index Theorem* relates the presence of zero-modes ($\lambda = 0$) in the spectrum of $\not{D}$ to the topological charge of the gluon field:

$$Q = n_0^{(+)} - n_0^{(-)}.$$

If configuration has $Q \neq 0$, lowest eigenvalues: $\lambda_{\mathrm{min}} = m_f$.

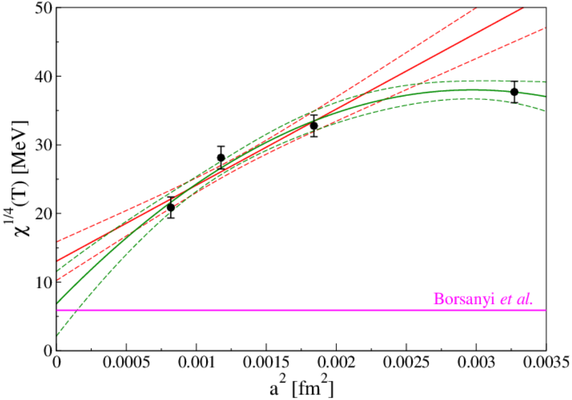
Typical lattice fermionic discretizations (e.g., Wilson, staggered) do not have exact zero-modes $\implies$ determinant fails to efficiently suppress configurations

$$\lambda_{\mathrm{min}} = m_f \longrightarrow m_f + i\lambda_0, \qquad \lambda_0 \underset{a \to 0}{\to} 0.$$

Large lattice artifacts at high T

Uneffective suppression of configuration $\Longrightarrow$ large cut-off effects at finite lattice spacing

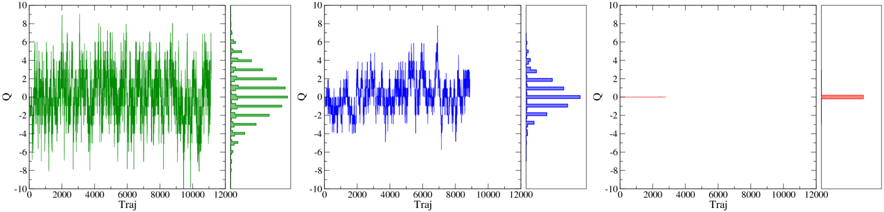
$\Longrightarrow$ continuum extrapolation not under control (Fig. Bonati et al., 2018):



Topological Critical Slowing Down (topological freezing)

Approaching the continuum limit $a \to 0$, standard algorithms (such as Hybrid Monte Carlo), becomes less and less ergodic.

This means that they become incapable of changing the topological charge of the configuration in a reasonable Monte Carlo time.



Left to right: $a \simeq 0.082$ fm, 0.057 fm and 0.040 fm (figs. Bonati et al., 2016)

In the continuum topological sectors are separated by infinite free-energy barriers: cannot change Q by local configuration updating.

Simulations on very fine lattice spacings are thus extremely challenging.

Reweighting + fixed-sector integral

Strategies outlined by BMW collab. to compute $\chi(T)$ (Borsanyi et al., 2016)

- **Reweighting**

  To restore the proper suppression due to Dirac zero-modes:

$$\chi = \frac{\langle Q^2 \rangle}{V} \longrightarrow \chi_{\text{rew}} = \frac{1}{V} \frac{\langle Q^2 w(Q) \rangle}{\langle w(Q) \rangle}, \qquad w(Q) = \prod_{f=1}^{N_f} \prod_{i=1}^{2|Q|} \left(\frac{m_f^2}{m_f^2 + \lambda_i^2} \right)^{\frac{1}{4}}$$

- **Fixed-sector integral**

  Assuming DIGA holds: $P_0 \gg P_1 \gg P_2 \implies \chi \simeq \dfrac{2}{V} \dfrac{P_1}{P_0}$

  Strategy to obtain P_1/P_0:

  - Perform simulations at fixed value of $Q = 0, 1$ and compute:

$$B_1 \equiv -\frac{d}{d \log T} \left(\frac{P_1}{P_0} \right) = -\left(\frac{d\beta}{d \log a} \right) \left(\langle S_g \rangle_1 - \langle S_g \rangle_0 \right), \qquad S_{\text{YM}}^{(L)} \equiv \beta S_g$$

  - compute $(P_1/P_0)(T_0)$ for a temperature T_0 where it is feasible for the simulation to naturally explore different topological sectors
  - compute $B_1(T')$ for several $T_0 < T' < T$
  - obtain $(P_1/P_0)(T)$ for the target temperature T via

$$\left(\frac{P_1}{P_0} \right)(T) = \left(\exp \left\{ \int_{T_0}^{T} d \log T' B_1(T') \right\} \right) \left(\frac{P_1}{P_0} \right)(T_0)$$

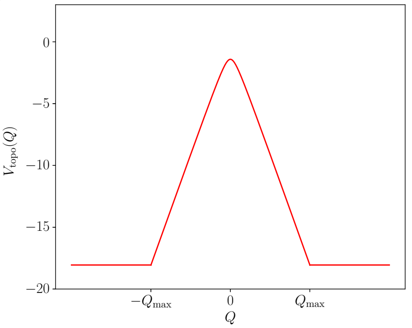
Multicanonical approach

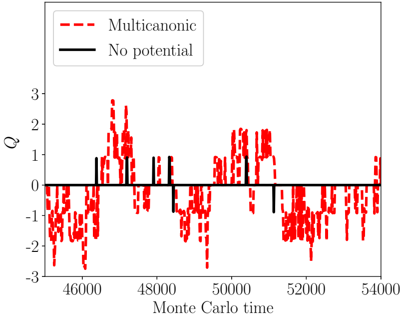
Multicanonic algorithm: add bias potential to the action to enhance the probability of visiting suppressed topological sectors (Jahn et al., 2018; Bonati et al., 2018)

$$S_{\rm QCD}^{(L)} \to S_{\rm QCD}^{(L)} + V_{\rm topo}(Q) \qquad \Longrightarrow \qquad P \propto e^{-S_{\rm QCD}^{(L)}} \to P_{\rm mc} \propto e^{-S_{\rm QCD}^{(L)}} e^{-V_{\rm topo}(Q)}$$

Mean values $\langle \mathcal{O} \rangle$ with respect to P recovered through reweighting:

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

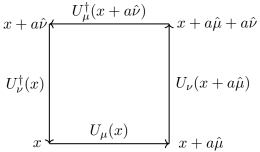




Fermionic definitions of the lattice topological charge

Simplest lattice discretization of the topological charge achieved via plaquette: gluonic lattice topological charge:

$$Q_{\text{gluo}} = \frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\sum_x \text{Tr}\left\{\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)\right\}$$



Improved gluonic discretizations can be built from $n \times m$ loops.

These discretizations know nothing of the chiral properties of fermions, which are tighty related to topology.

Large cut-off effects affecting χ_{gluo} may be reduced adopting a fermion definition, based on the Index Theorem.

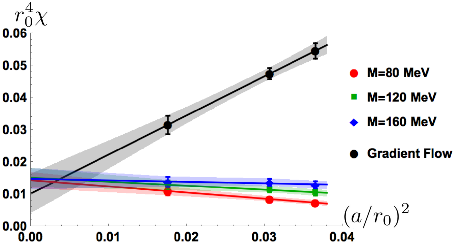


Fig. from Alexandrou et al., 2017 at zero temperature: improved scaling towards the continuum with fermionic definition of χ compared to standard gluonic definition.

Fermionic topological susceptibility: two examples

Index Theorem: $Q = n_0^{(+)} - n_0^{(-)} = \mathrm{Tr}(\gamma_5)$

$$\begin{aligned} \not{D} u_\lambda &= i\lambda u_\lambda, \qquad & \not{D}\gamma_5 = \gamma_5 \not{D}^\dagger = -\gamma_5 \not{D} \\ \not{D}\gamma_5 u_\lambda &= -i\lambda\gamma_5 u_\lambda \qquad & \Longrightarrow \; u_\lambda^\dagger \gamma_5 u_\lambda = \delta_{\lambda 0} \end{aligned}$$

- Chiral Susceptibility $\to Q = m\,\mathrm{Tr}\left\{\gamma_5(\not{D}+m)^{-1}\right\}$

$$\chi = \frac{m^2}{V}\left\langle\left(\mathrm{Tr}\left\{\gamma_5(\not{D}+m)^{-1}\right\}\right)^2\right\rangle \equiv m^2 \chi_5^{(\mathrm{disc})}$$

On the lattice $\chi_5^{(\mathrm{disc})}$ is measured via the disconnected chiral susceptibility $\chi^{(\mathrm{disc})}$ assuming $\mathrm{U}(1)_\mathrm{A}$ is restored (Petreckzy et al. 2016; Lombardo et al., 2020):

$$\chi_5^{(\mathrm{disc})} = \chi^{(\mathrm{disc})} = \frac{1}{V}\langle(\mathrm{Tr}\left\{(\not{D}+m)^{-1}\right\})^2\rangle - (\langle\mathrm{Tr}\left\{(\not{D}+m)^{-1}\right\}\rangle)^2$$

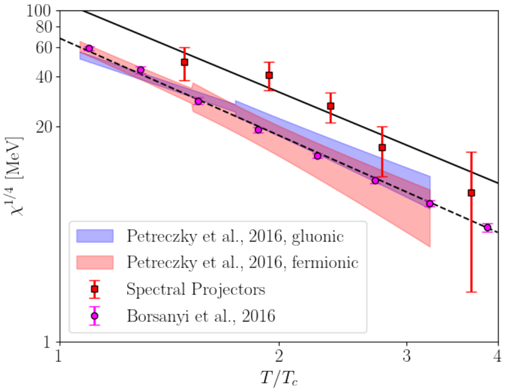
- Spectral Projectors $\to Q = \sum_{\lambda=0} u_\lambda^\dagger \gamma_5 u_\lambda$

On the lattice, extend sum up to $\lambda \le M$ if fermions break chiral symmetry

$$Q_{\mathrm{SP}} = \sum_{\lambda\le M} u_\lambda^\dagger \gamma_5 u_\lambda = \mathrm{Tr}\left\{\gamma_5 \mathbb{P}_M\right\}, \quad \mathbb{P}_M = \sum_{\lambda \le M} u_\lambda u_\lambda^\dagger$$

$$\chi_{\mathrm{SP}} = Z_{\mathrm{SP}}^2 \frac{\langle Q_{\mathrm{SP}}^2\rangle}{V}, \quad Z_{\mathrm{SP}}^2 = \frac{\langle \nu(M)\rangle}{\langle \mathrm{Tr}\{(\gamma_5\mathbb{P}_M)^2\}\rangle}$$

Lattice QCD results for $\chi(T)$



QCD with $N_f = 2+1$

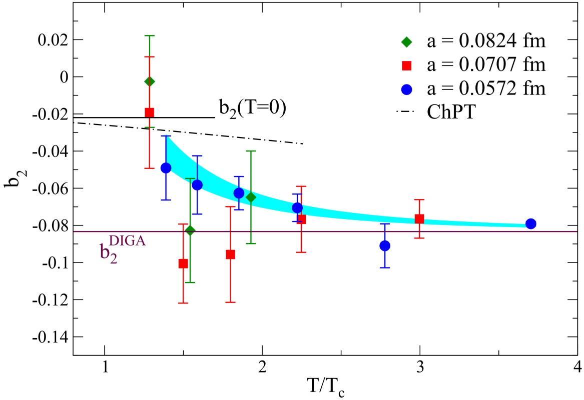
$$\chi^{1/4}_{\mathrm{DIGA}}(T) \sim (T_c/T)^2$$

Fig. adapted from Athenodorou, CB et al., 2022

Common qualitative agreement that a DIGA-like power-law sets in for $T \gtrsim 300$ MeV can be observed among different determinations.

Clear common qualitative agreement still to be achieved, in particular for $300 \text{ MeV} \lesssim T \lesssim 400$ MeV (see also Kotov, Trunin, Lombardo, 2020 for a similar discussion).

Lattice QCD results for $b_2(T)$



$$b_2 = -\frac{1}{12}\frac{\langle Q^4\rangle - 3\langle Q^2\rangle^2}{\langle Q^2\rangle}$$

(Fig. from Bonati et al., 2016)

Lattice determinations for $T > T_c$ approach the DIGA $b_2^{(\mathrm{DIGA})} = -1/12$, but deviations are visible (for the finest lattice spacing) up to $T \sim 300 - 350$ MeV. Agreeing findings in other recent works (e.g., Lombardo et al., 2020)

It would be interesting to provide controlled continuum extrapolations of b_2 in the shown temperature range.

Conclusions

Take-home messages

- Topology and θ-dependence in QCD related both to intriguing non-perturbative theoretical aspects (phase diagram, CP-violation, fermion chiral properties) and to phenomenology (e.g., PQ axion)
- Axions are promising candidates to simultaneously solve the strong-CP problem and explain (part of) observed Dark Matter
- Theoretical bounds on axion cosmology can be precisely assessed from the computation of $\chi(T)$ at high T in QCD by *misalignement*
- Lattice non-perturbative computation of $\chi(T)$ needed to gain full control over these predictions but several nontrivial computational problems have to be faced
- Several different works computed $\chi(T)$ in QCD during the last years with different strategies: complete quantitative agreement still lacking

Future outlooks

- Current main obstacle: topological critical slowing down (finer lattice spacing and/or higher temperatures)
- Several proposals, expected major improvements in the next years: Parallel Tempering on Boundary Conditions (Hasenbusch, 2017, CB et al., 2021, CB et al., 2022), machine-learning Equivariant Flows (Kanwar et al., 2020), Density of States method (Cossu et al., 2021).