θ-dependence in QCD and QCD-like theories from lattice simulations

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The presence of configurations with non-trivial topology, labelled by an integer winding number $Q = \int d^4x\ q(x)$, characterizes many non-perturbative properties of QCD

$$q(x) = \frac{g^2}{64\pi^2} G^a_{\mu\nu}(x)\tilde{G}^a_{\mu\nu}(x) = \frac{g^2}{64\pi^2}\epsilon_{\mu\nu\rho\sigma} G^a_{\mu\nu}(x) G^a_{\rho\sigma}(x)$$

$$GG \propto \vec{E}^a \cdot \vec{E}^a + \vec{B}^a \cdot \vec{B}^a \ ; \quad G\tilde{G} \propto \vec{E}^a \cdot \vec{B}^a$$

$G\tilde{G}$ **is renormalizable and a possibile coupling to it is a free parameter of QCD**

$$Z(\theta) = \int [\mathcal{D}A][\mathcal{D}\bar{\psi}][\mathcal{D}\psi]\ e^{-S_{QCD}}\ e^{i\theta Q}$$

the theory at $\theta \neq 0$ is well defined, but presents explicit breaking of CP symmetry.

$|\theta| < 10^{-10}$ **(strong CP-problem)**

however θ-dependence is related to essential aspects of strong interactions anyway

and to BSM physics too (axion cosmology)

QCD at non-zero θ

The free energy density $f(\theta) = -T \log Z/V$ is a periodic even function of θ

It is connected to the probability distribution $P(Q)$ at $\theta = 0$ via Taylor expansion:

$$f(\theta) - f(0) = \frac{1}{2} f^{(2)} \theta^2 + \frac{1}{4!} f^{(4)} \theta^4 + \ldots \quad ; \qquad f^{(2n)} = \left. \frac{d^{2n} f}{d\theta^{2n}} \right|_{\theta=0} = -(-1)^n \frac{\langle Q^{2n} \rangle_c}{V}$$

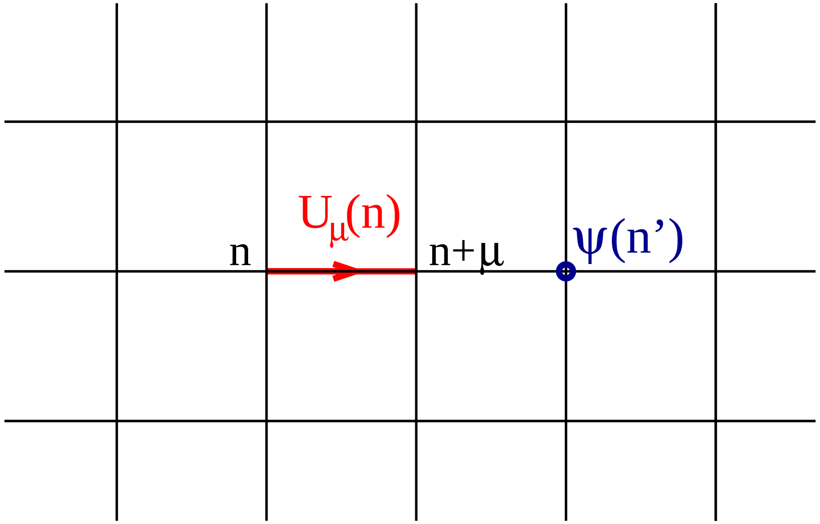
A common parametrization is the following

$$f(\theta, T) - f(0, T) = \frac{1}{2} \chi(T) \theta^2 \left(1 + b_2(T) \theta^2 + b_4(T) \theta^4 + \cdots \right)$$

$$\chi = \frac{1}{V} \langle Q^2 \rangle_0 = f^{(2)} \qquad b_2 = - \left. \frac{\langle Q^4 \rangle - 3 \langle Q^2 \rangle^2}{12 \langle Q^2 \rangle} \right|_{\theta=0} \qquad b_4 = \left. \frac{\langle Q^6 \rangle - 15 \langle Q^4 \rangle \langle Q^2 \rangle + 30 \langle Q^2 \rangle^3}{360 \langle Q^2 \rangle} \right|_{\theta=0}$$

$P(Q)$ is non-perturbative: a lattice investigation is the ideal first-principle approach

θ-dependence from Lattice QCD simulations



Gauge fields are 3×3 unitary complex matrixes living on lattice links (link variables)

$$U_\mu(n) \simeq \mathcal{P} \exp\left(ig \int_n^{n+\mu} A_\mu dx_\mu\right)$$

Fermion fields live on lattice sites

$$Z(V,T) = \mathrm{Tr}\left(e^{-\frac{H_{\rm QCD}}{T}}\right) \Rightarrow \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi} e^{-(S_G[U]+\bar{\psi}M[U]\psi)} = \int \mathcal{D}U e^{-S_G[U]} \det M[U]$$

$$T = \frac{1}{\tau} = \frac{1}{N_t a(\beta, m)}$$

τ **is the extension of the compactified time**

Main Technical and Numerical Problems in Lattice QCD simulations

- topological charge renormalizes, naive lattice discretizations are non-integer valued
  - gluonic definitions standard lattice discretization of $G\tilde{G}$
  - fermionic definitions compute Q from the index theorem: $Q = \mathrm{Tr}\{\gamma_5\} = \mathrm{Index}(D) = n_+ - n_-$
  - renormalize or smooth gauge fields: compute multiplicative an additive renormalizations to cumulants, or make use of various techniques to smooth gauge fields and recover integer Q

  All methods lead to consistent results in the continuum limit.

  The impact of $O(a^2)$ corrections can change.

- Sign problem at $\theta \neq 0$

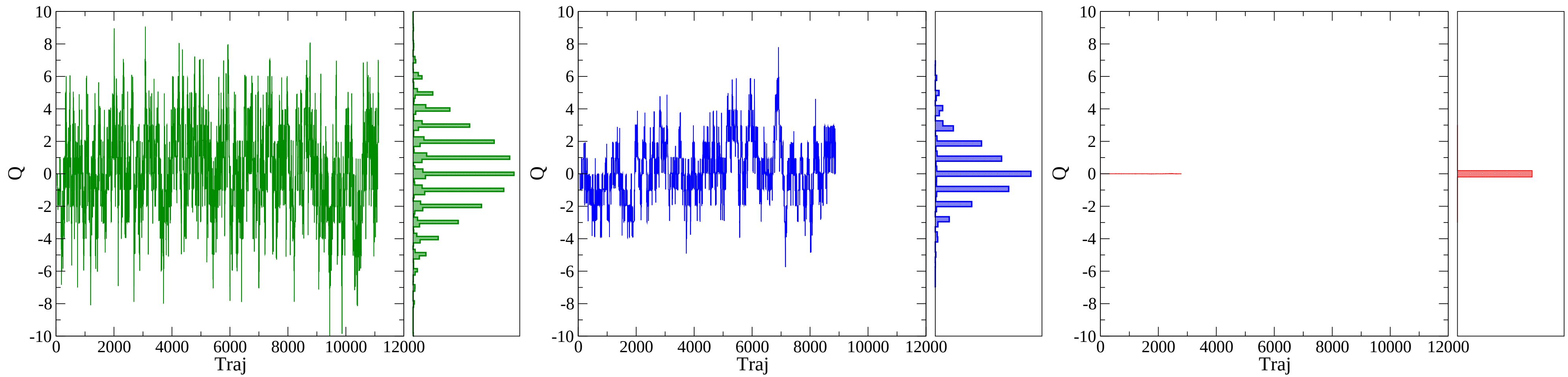
  Taylor expansion from cumulants at $\theta = 0$, in principle $\theta \neq 0$ not needed

  but explicit source improves signal/noise ratio $\Longrightarrow$ simulations at imaginary θ

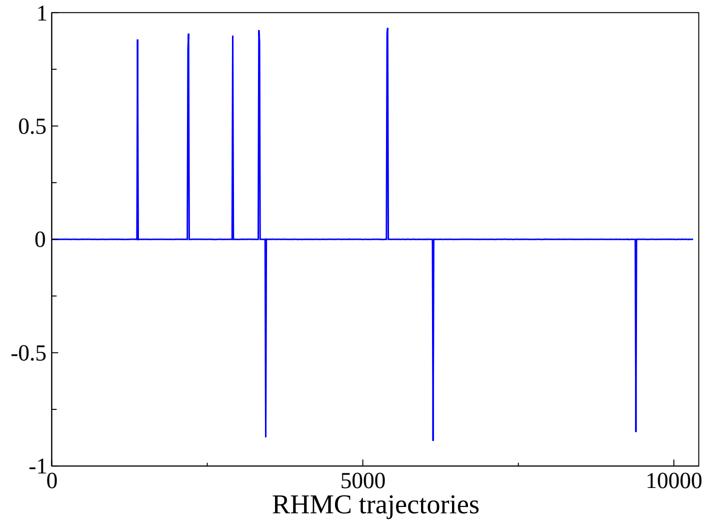
- Finally, various algorithmic problems can affect:
  - Loss of ergodicity (freezing) in the continuum limit
  - Need to sample very rare events when $\chi V = \langle Q^2 \rangle \ll 1$

Evolution of Q in Monte-Carlo time for decreasing lattice spacings (from left to right)

C. Bonati et al., JHEP 1603 (2016) 155 $\quad N_f = 2+1$ **QCD with physical quark masses**



Evolution of Q in MC time for an high T simulation of $N_f = 2+1$ QCD, $\langle Q^2 \rangle \sim 0.01$.



In presence of light fermions, the impact of $O(a^2)$ corrections to the continuum limit can be much worse

$$Z(V,T) = \mathrm{Tr}\left(e^{-\frac{H_{\mathrm{QCD}}}{T}}\right) \Rightarrow \int \mathcal{D}U e^{-S_G[U]} \det M[U]$$

$$M \sim D + m_q$$

$Q \neq 0 \implies$ **zero modes of** $D \implies \det M$ **suppresses topological fluctuations and** θ**-dependence as** $m_q \to 0$

However, if the lattice discretization of M has poor chiral properties, $\det M$ will fail its task and let many more $Q \neq 0$ configurations in than it should.

Lattice computations vs analytic predictions

Lattice computations can be useful by themselves, by they are especially useful when compared to analytic predictions valid in particular approximation schemes: Large-N expansion, Dilute Instanton Gas Approximation (DIGA), Chiral Perturbation Theory (χPT), ...

That helps understanding the validity of the approximation scheme and, as a consequence, gives more information about the non-perturbative structure of strong interactions

In the following I will review some recent results in pure gauge and full QCD with a focus on this aspect

Predictions about θ-dependence - large-N expansion

Large-N_c for low T $SU(N_c)$ gauge theories (Witten, 1980)

$g^2 N_c = \lambda$ **fixed as** $N_c \to \infty$ $\Longrightarrow$ **Effective instanton weight** $e^{-8\pi^2 N_c/g^2} \to 0$

Non-trivial θ-dependence persists only if the dependence is on $\bar{\theta} = \theta/N_c$.

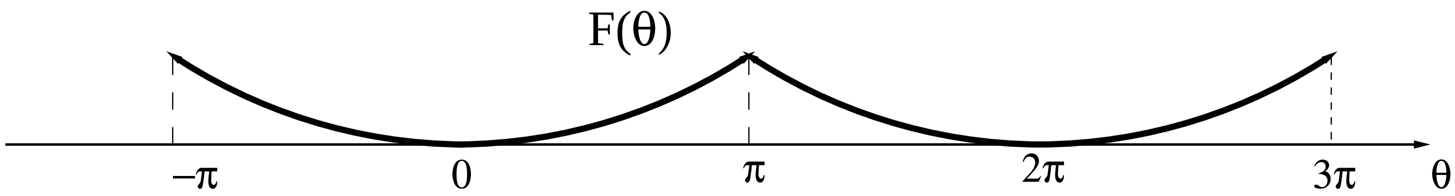
$$f(\theta, T) - f(0, T) = N_c^2 \bar{f}(\bar{\theta}, T)$$

$$\bar{f}(\bar{\theta}, T) = \frac{1}{2}\bar{\chi}\bar{\theta}^2 \left[1 + \bar{b}_2\bar{\theta}^2 + \bar{b}_4\bar{\theta}^4 + \cdots\right]$$

Matching powers of $\bar{\theta}$ and θ we obtain

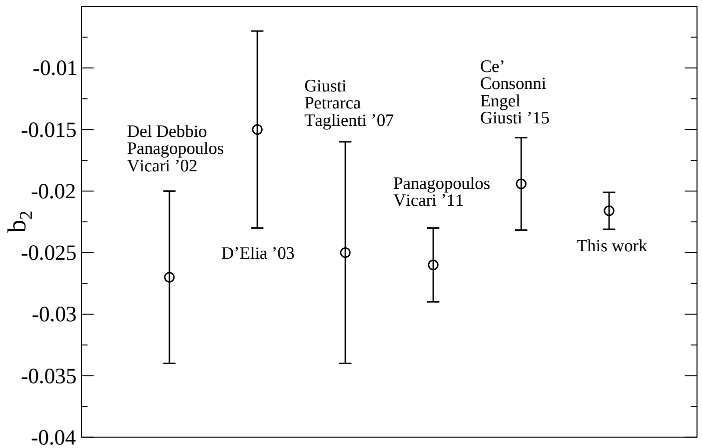
$$\chi \sim N_c^0 \sim (180\,\mathrm{MeV})^4 \ \ (\mathrm{Witten-Veneziano}) \ ; \quad b_2 \sim N_c^{-2} \ ; \quad b_{2n} \sim N_c^{-2n}$$

$P(Q)$ is purely Gaussian in the large N_c limit.

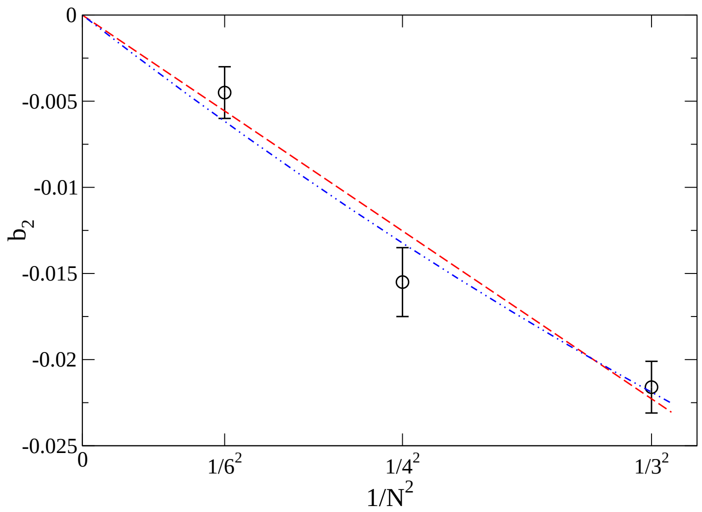


Pure gauge lattice results: $T = 0$ (Yang-Mills vacuum)

Topological susceptibility well known since many years, has a finite large-N limit, and compatible with the Witten-Veneziano mechanism for $m_{\eta'}$, $\chi^{1/4} \sim 180$ MeV



Determination of b_2 more difficult. Most recent determination for $SU(3)$ (Bonati, MD, Scapellato, 1512.01544) obtained by introducing an external imaginary θ source to improve signal/noise.



Clear evidence for the predicted large-N_c scaling of b_2:

$$b_2 \simeq \frac{\bar{b}_2}{N^2}$$

with $\bar{b}_2 = -0.20(2)$

(Bonati, MD, Rossi, Vicari, 1607.06360)

In some QCD-like theories, large-N is quantitative: $2d\, CP^{N-1}$ models

$\chi = \bar{\chi} N^{-1} + O(N^{-2})$ **and** $b_{2n} = \bar{b}_{2n} N^{-2n} + O(N^{-2n-1})$.

$$\xi^2 \chi = \frac{1}{2\pi N} + \frac{e_2}{N^2} + O\left(\frac{1}{N^3}\right) \;, \quad e_2 = -0.0605 \;; \quad \xi = 2^{nd}\,\text{moment corr. length}$$

$$b_2 = -\frac{27}{5}\frac{1}{N^2} + O\left(\frac{1}{N^3}\right) \;, \quad b_4 = -\frac{25338}{175}\frac{1}{N^4} + O\left(\frac{1}{N^5}\right) \;,$$

LO χ: Luscher, PLB 78, 465 (1978) D'Adda, Luscher, Di Vecchia, NPB 146, 63 (1978), Witten, NPB 149, 285 (1979)

NLO χ (e_2): M. Campostrini and P. Rossi, PLB 272, 305 (1991).

LO b_2: L. Del Debbio, G. M. Manca, H. Panagopoulos, A. Skouroupathis, E. Vicari, JHEP 0606, 005 (2006)

LO all b_{2n}: P. Rossi, PRD 94, 045013 (2016) C. Bonati, MD, P. Rossi, E. Vicari, PRD 94, 085017 (2016)

Lattice checks till 2017:

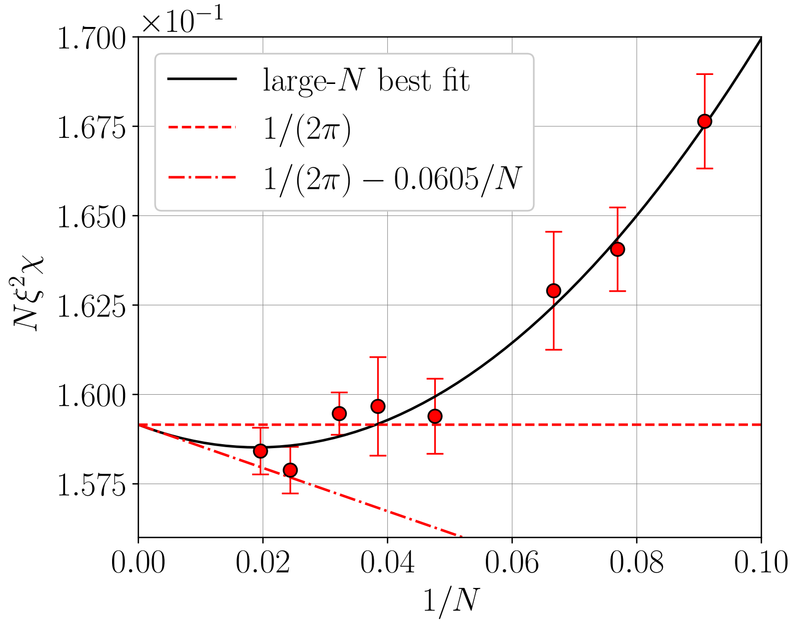
LO χ: OK; **NLO χ: disagreement even in sign;** **LO b_2: never tried**

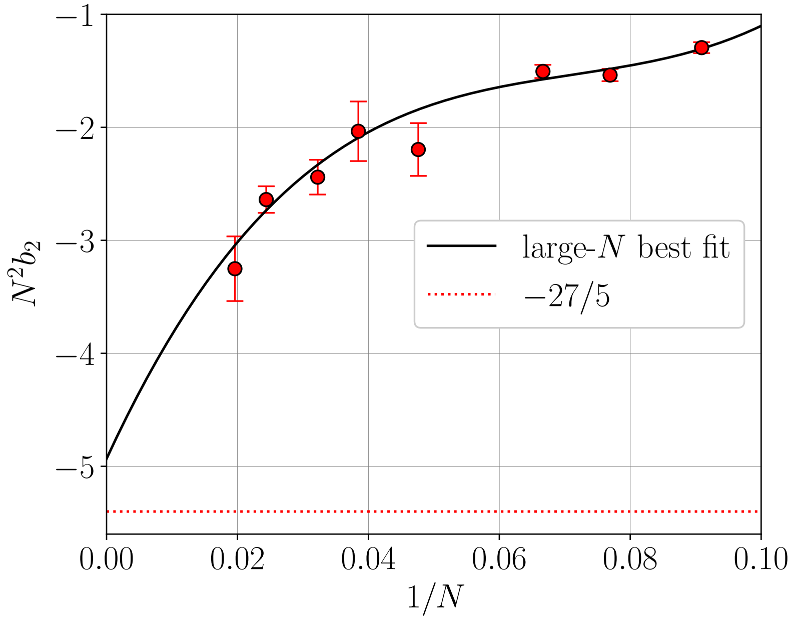
M. Campostrini, P. Rossi and E. Vicari, PRD 46, 2647 (1992) E. Vicari, PLB 309, 139 (1993) L. Del Debbio, G. M. Manca and E. Vicari, PLB 594, 315 (2004) J. Flynn, A. Juttner, A. Lawson and F. Sanfilippo, arXiv:1504.06292 M. Hasenbusch, PRD 96, no. 5, 054504 (2017)

MAIN LIMITATION: critical slowing down of Q for large N

This year update: **M. Berni, C. Bonanno, MD, in progress ...**

C. Bonanno, C. Bonati, MD, JHEP 1901, 003 (2019)





- **Thanks to a new algorithm** **(M. Hasenbusch, arXiv:1706.04443)**: **we reach up to** $N = 51$

- **results for** χ **(left):** $\xi^2\chi = 1/(2\pi N) + e_2/N^2 + e_3/N^3$

  $e_2 = -0.066(13)$; $e_3 = 1.75(20)$; $\tilde{\chi}^2 = 0.5$

- **results for** b_2 **(right):** $b_2 = p_2/N^2 + p_3/N^3 + p_4/N^4 + p_5/N^5$

  $p_2 = -4.9(1.1)$; $p_3 = 125(67)$; $p_4 = -1600(1000)$; $p_5 = -7700(6000)$; $\tilde{\chi}^2 = 1.6$

- **Conclusions:** **NLO for** χ **and LO for** b_2 **successfully checked; NNLO for** χ **and NLO for** b_2 **predicted;** **slow** $1/N$ **convergence, due to singularity at** $N = 2$**??**

Predictions about θ-dependence - DIGA

Dilute Instanton Gas Approximation (Gross, Pisarski, Yaffe 1981)

IDEA: semi-classical integration around classical solutions with $Q \neq 0$: instantons

1-loop one-instanton contribution finite for finite N $\propto \exp\left(-\frac{8\pi^2}{g^2(\rho)}\right)$

- ρ is the instanton radius: works well for small ρ, breaks down for $\rho^{-1} \lesssim \Lambda_{QCD}$
- Finite-T acts as an IR cut-off to ρ, making the 1-loop result more and more reliable
- top. fluctuations exponentially suppressed $\Longrightarrow$ dilute instanton gas approximation

DIGA predictions

- **instantons - antiinstantons treated as uncorrelated (non-interacting) objects**
  Poisson distribution with an average probability density p per unit volume

$$Z_\theta \simeq \sum \frac{1}{n_+! n_-!} (V_4 p)^{n_+ + n_-} e^{i\theta(n_+ - n_-)} = \exp\left[2V_4 p \cos\theta\right]$$

$$F(\theta,T) - F(0,T) \simeq \chi(T)(1-\cos\theta) \implies \quad b_2 = -1/12\,; \quad b_4 = 1/360\,; \ldots$$

independent of N

- **The prefactor $\chi(T)$ can also be computed in the 1-loop approximation:**

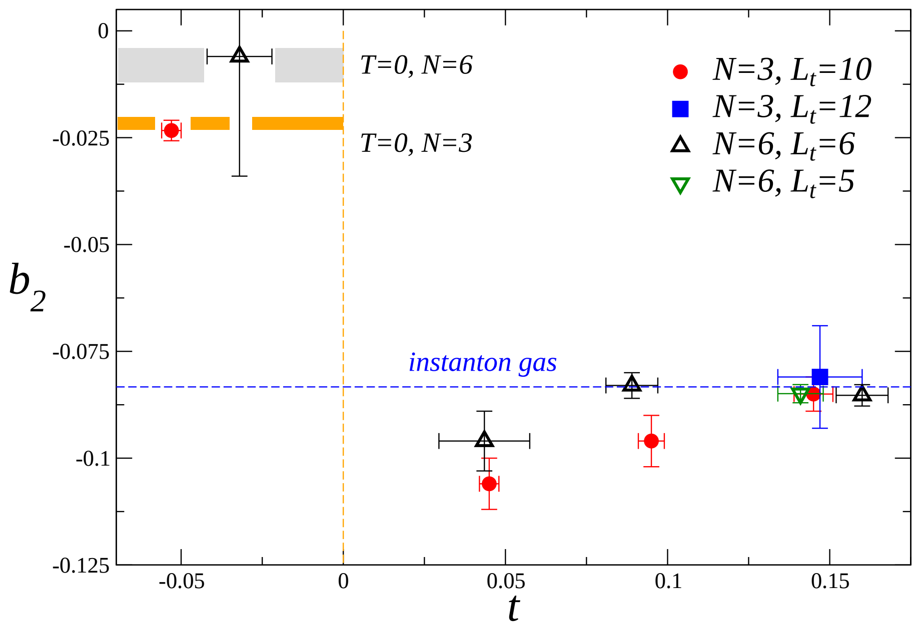
$$\chi(T) \sim T^4 \left(\frac{m}{T}\right)^{N_f} e^{-8\pi^2/g^2(T)} \sim m^{N_f} T^{4-\frac{11}{3}N_c - \frac{1}{3}N_f}$$

At some T one should cross from large-N to DIGA. How high T?

Notice: the $(1-\cos\theta)$ prediction is just related to diluteness and might be good before reaching the asymptotic perturbative behavior

Pure gauge lattice results: Finite T, across and above T_c

χ **drops suddenly after** T_c, **known since many years** (B. Alles, MD, A. Di Giacomo, hep-lat/9605013)



from Bonati, MD, Panagopoulos, Vicari 1301.7640

DIGA values for higher cumulants reached quite soon, already for $T \gtrsim 1.1\, T_c$.

Emerging picture:

- **shortly after deconfinement (breaking of center symmetry), topological excitations behave as a dilute non-interacting gas, DIGA:** $f(\theta) \propto (1 - \cos(\theta))$.
- **The change of regime seems quite abrupt, localized around** T_c, **and sharper and sharper as** N **increases**

A closer look at the relation between center symmetry and θ-dependence

Is it possible to preserve Z_N center symmetry, even with a small compactification radius (high-T, small coupling), by deforming the pure Yang-Mills action?

M. Unsal and L. Yaffe: PRD 78, (2008) 065035

J.C. Myers and C. Ogilvie: PRD 77, (2008) 125030 (first lattice study)

$$S^{def} = S_{YM} + h \sum_{\vec{n}} |TrP(\vec{n})|^2$$

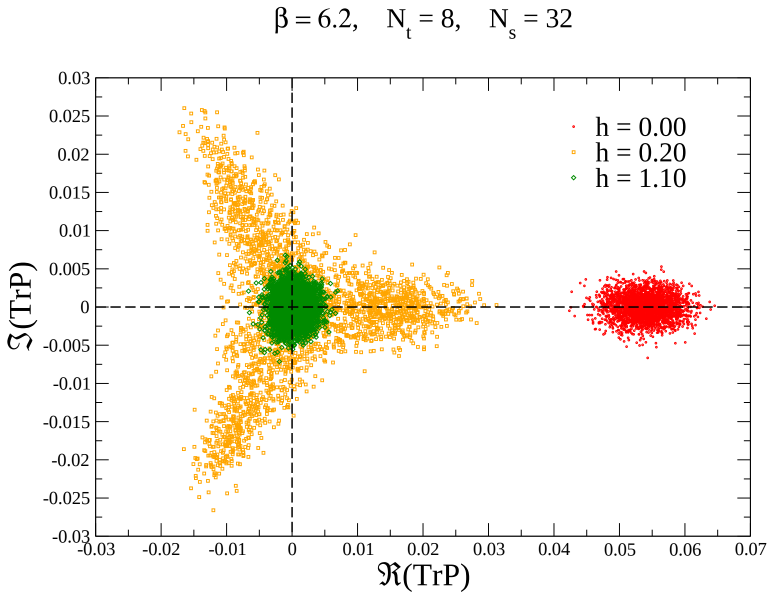
$SU(3)$: just one deformation, suppresses large values of $|TrP(\vec{n})|$ locally $\Longrightarrow$ for large enough h, center symmetry is restored even at high-T (small coupling)

QUESTION: **what happens to θ dependence?**

What is DIGA related to? Small coupling or broken center symmetry?

Lattice results $\Longrightarrow$ C. Bonati, M. Cardinali, MD, PRD 98, 054508 (2018), arXiv:1807.06558

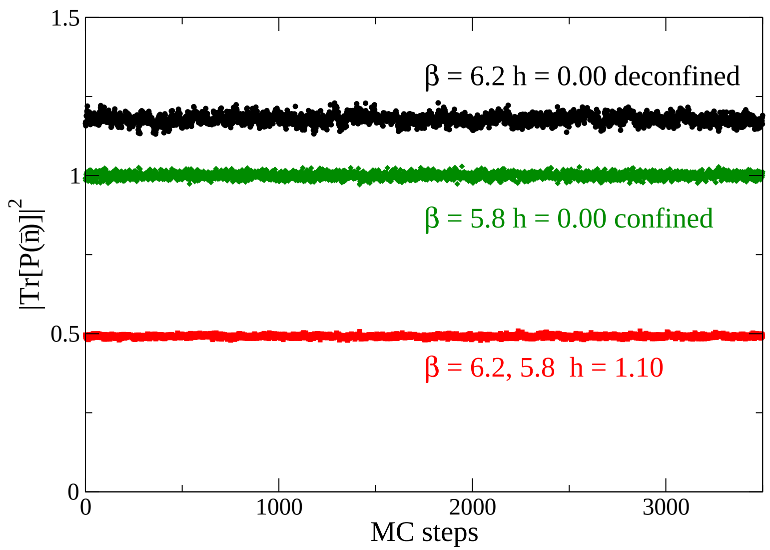
Restoration of Z_3 takes place in a non-trivial way



- $T \simeq 1.4\, T_c$, **broken** Z_3 **at** $h = 0$

- **Center symmetry recovered by increasing** h

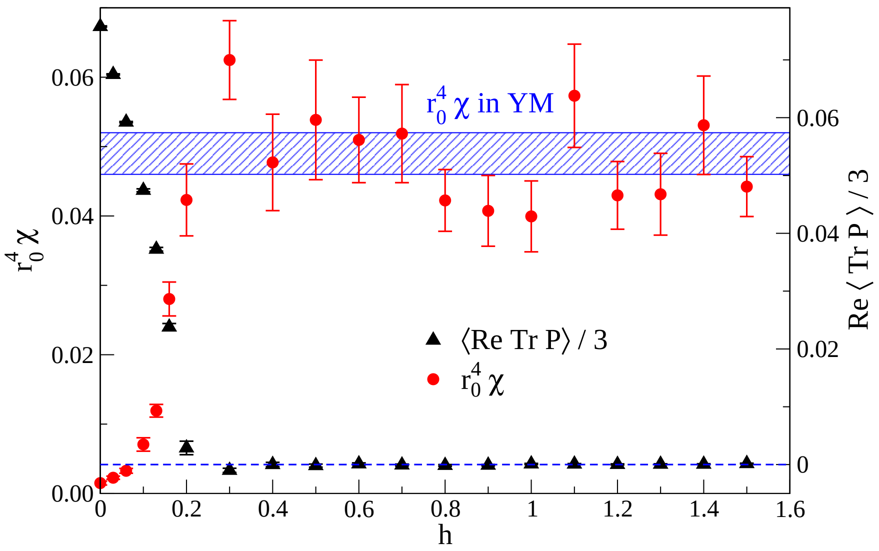
- **Some differences from the standard confined phase emerge looking at the adjoint Polyakov loop**

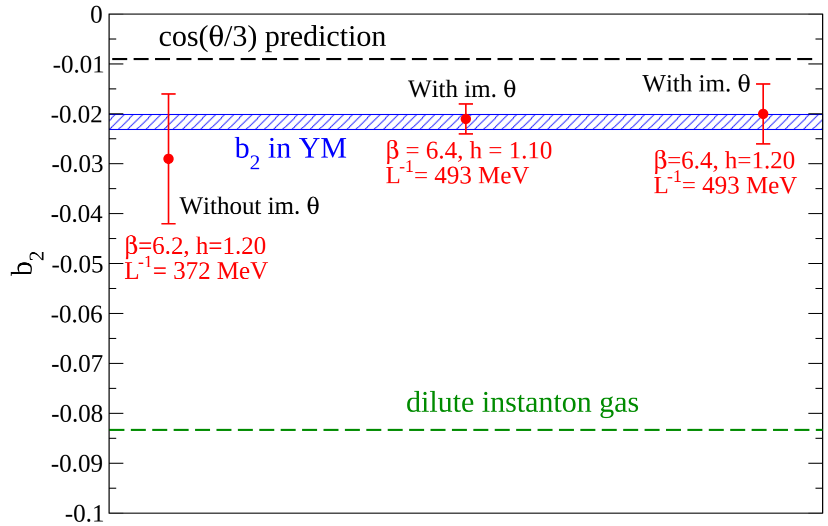


$$P^{adj} = |TrP|^2 - 1$$

a negative value of P^{adj} **means that** $|TrP|$ **tends to vanish locally (point by point).**

For $T < T_c$ **it vanishes by long-range disorder**





θ-dependence seems to be sensible just to the restoration of center symmetry (either locally or by long-range disorder)

- **Left:** the topological susceptibility goes back to its $T = 0$ value
- **Right:** the same happens for b_2.

Notice: semiclassical arguments (Unsal, Yaffe, 2008) predict $b_2 = -1/(12N_c^2)$ (Fractional Instanton Gas Approximation) This is still not observed at the explored L^{-1}

significantly smaller compactification radii are still hard for lattice

Can corrections to leading semiclassical be computed?

Better insight by going to $N > 3$

C. Bonati, M. Cardinali, MD, F. Mazziotti, in progress

$SU(4)$: center symmetry has two possible breaking patterns

$$Z_4 \to \mathrm{Id} \;\; ; \quad Z_4 \to Z_2$$

Complete restoration of Z_4 requires the vanishing of two traces: P and P^2

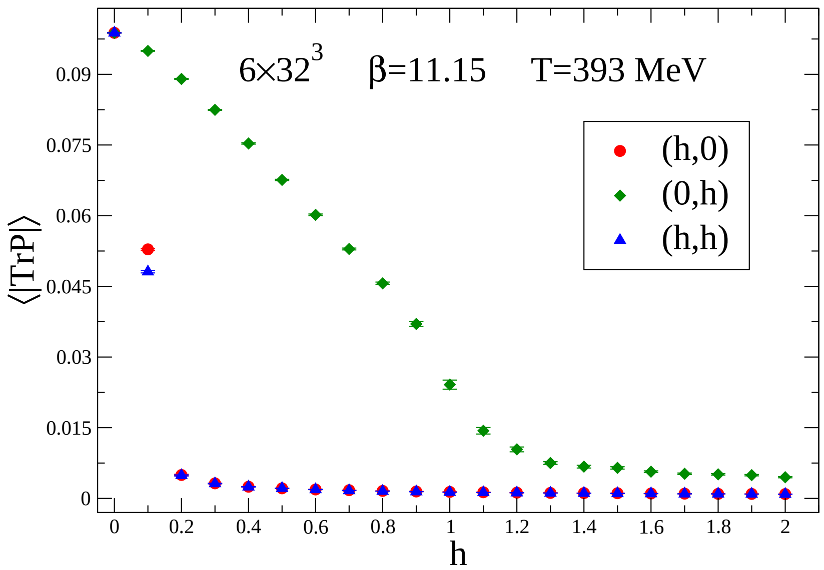
two possible trace deformations to be added to the action

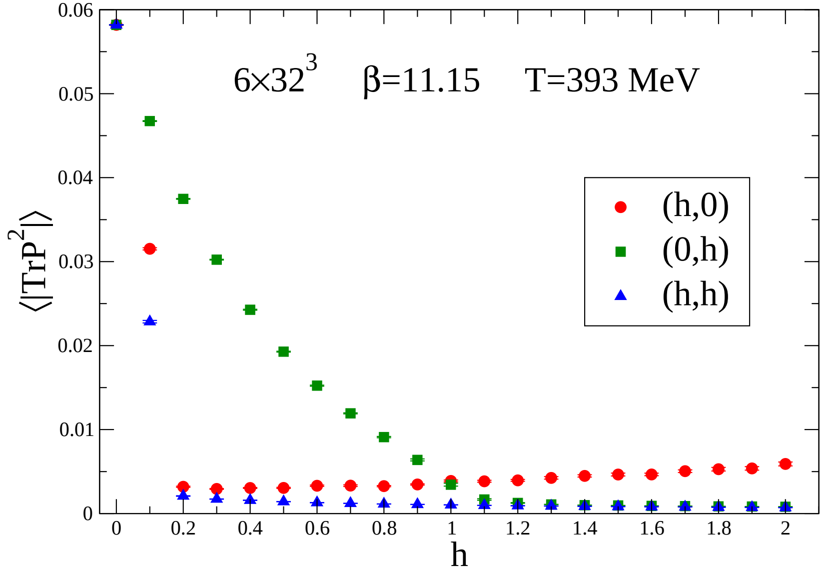
$$S^{def} = S_{YM} + h_1 \sum_{\vec{n}} |TrP(\vec{n})|^2 + h_2 \sum_{\vec{n}} |TrP^2(\vec{n})|^2$$

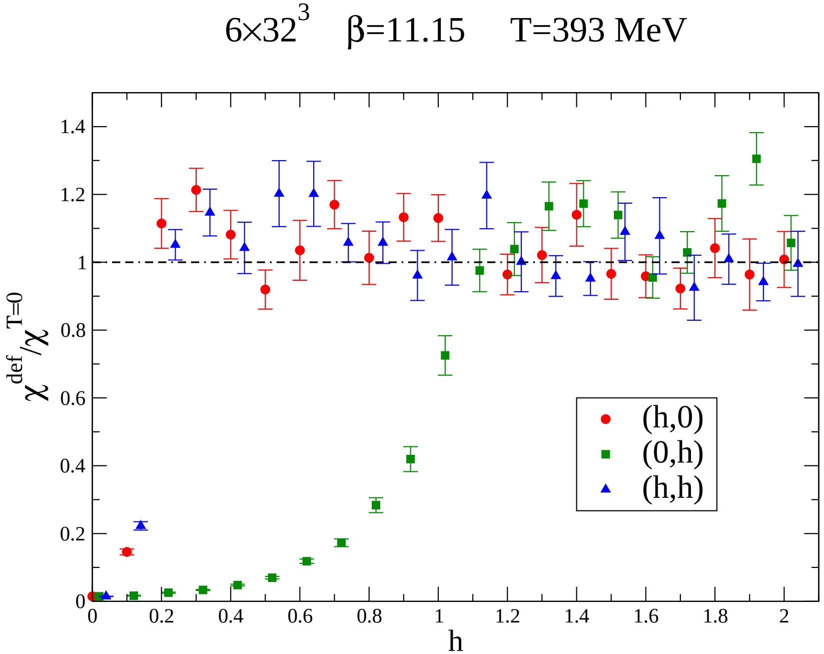
What about θ-dependence?

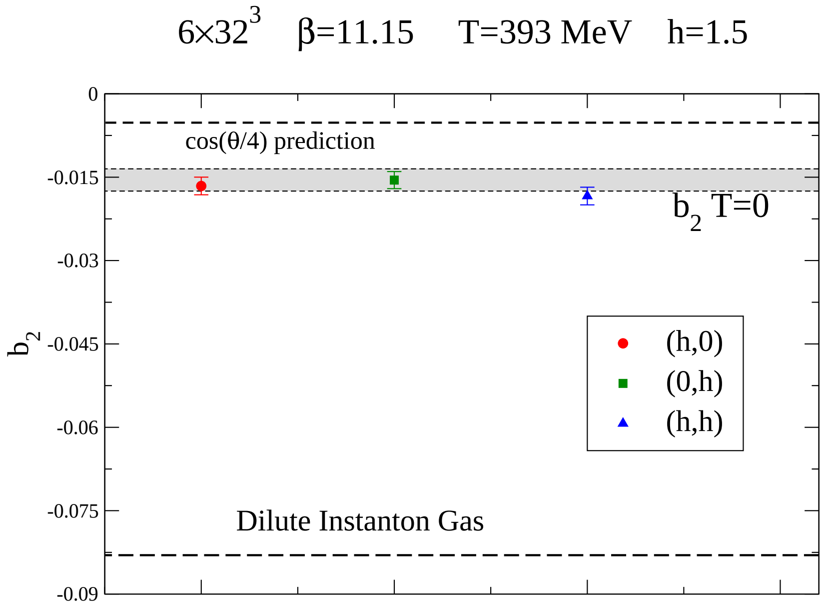
Is it sensitive to partial or complete restoration?

ANSWER: θ-dependence back to confined values only for complete restoration









Predictions about θ-dependence - χPT

Chiral Perturbation Theory for QCD with light quarks at low T

In the presence of quarks, θ can be moved to light quark masses (if any!) by $U(1)$ axial rotations. Then, at low T, χPT can be applied as usual.

Di Vecchia, Veneziano 1980, G. G. di Cortona, E. Hardy, J. P. Vega and G. Villadoro, 1511.02867

Result for the ground state energy

$$E_0(\theta) = -m_\pi^2 f_\pi^2 \sqrt{1 - \frac{4 m_u m_d}{(m_u + m_d)^2} \sin^2 \frac{\theta}{2}}$$

$$\chi = \frac{z}{(1+z)^2} m_\pi^2 f_\pi^2, \quad b_2 = -\frac{1}{12} \frac{1+z^3}{(1+z)^3}, \quad z = \frac{m_u}{m_d}$$

Explicitly

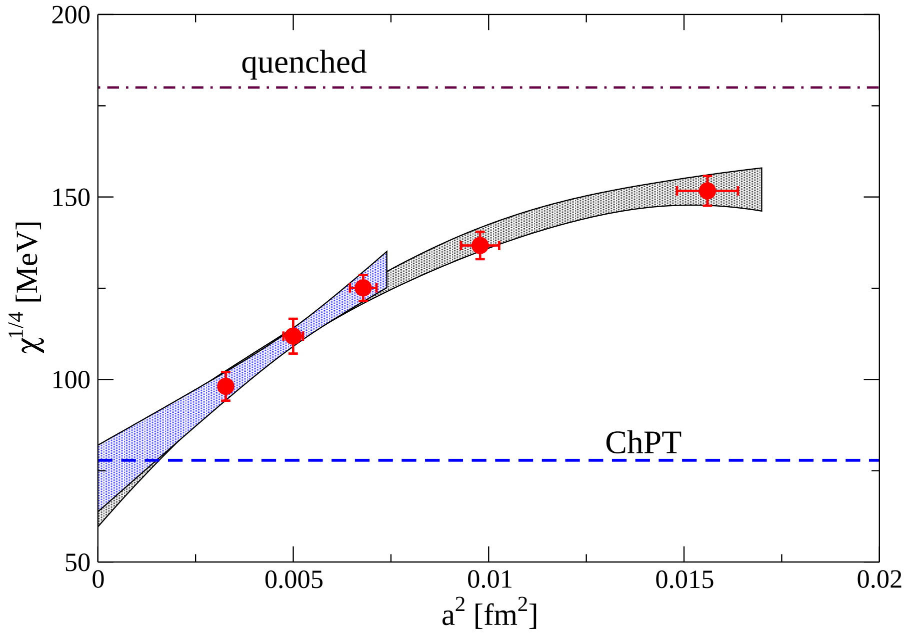
$$z = 0.48(3) \qquad \chi^{1/4} = 75.5(5)\,\mathrm{MeV} \qquad b_2 = -0.029(2)$$

$$z = 1 \qquad \chi^{1/4} = 77.8(4)\,\mathrm{MeV} \qquad b_2 = -0.022(1)$$

Lattice results for full QCD at $T = 0$

C. Bonati, MD, M. Mariti, G. Martinelli, M. Mesiti, F. Negro, F. Sanfilippo and G. Villadoro, 1512.06746

$N_f = 2 + 1$ **QCD, physical quark masses, improved staggered fermions**



The approach to the continuum limit is quite slow and lattice spacing well below 0.1 fm are needed

continuum limit compatible with ChPT

no results yet available for b_2

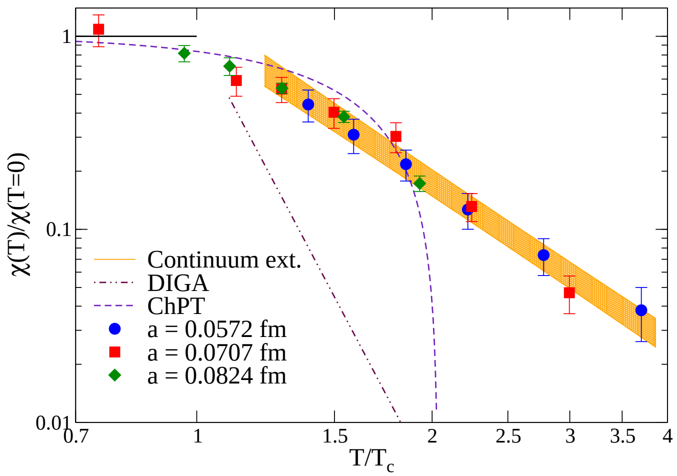
slow approach to continuum $\leftrightarrow$ slow approach to chiral properties of fermion fields

zero modes are not exact, $\det M$ does not properly suppress $Q \neq 0$ configurations, $\langle Q^2 \rangle$ is still one order of magnitude larger than expected at $a \sim 0.1$ fm

Finite T results for $N_f = 2+1$ QCD

χ **is related to the QCD axion mass:** $m_a^2 = \chi / f_a^2$

T-dependence of $\chi(T)$ fixes cosmological axion abundancies, and, by dark matter bounds, the value of f_a and of the axion mass today.



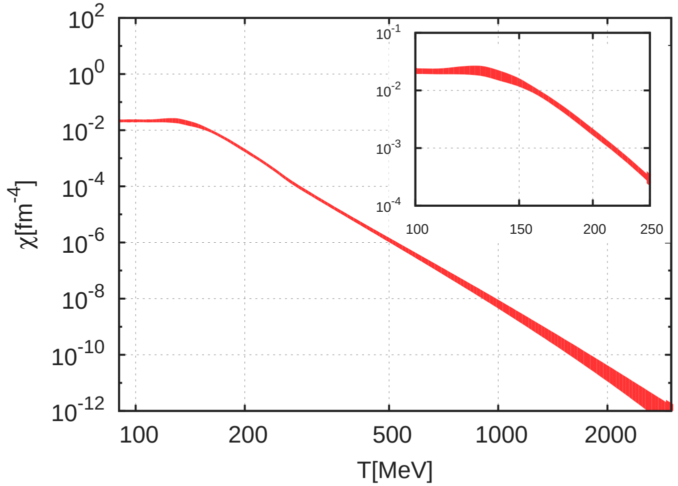
results from C. Bonati et al., 1512.06746

drop of χ much smoother than DIGA prediction:

$\chi(T) \propto 1/T^b$ **with** $b = 2.90(65)$ **(DIGA:** $b = 7.66 \div 8$**)**

results in a larger f_a, hence a smaller $m_a \sim$ 10 μeV

Finite a corrections seemed under control ...

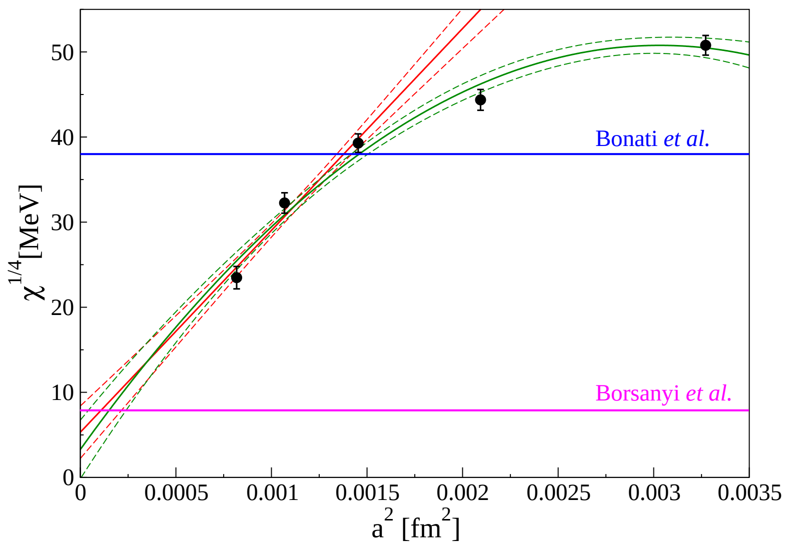


Later numerical results, based on finer lattice spacings, pointed to a much better agreement with DIGA, hence to higher $m_a \sim$ 100 μeV

Results from S. Borsanyi *et al.*, arXiv:1606.07494

Recently, we managed to reach much smaller lattice spacings (down to $a \sim 0.03$ fm) by means of an improved MC sampling (multicanonical algorithm)

C. Bonati, MD, G. Martinelli, F. Negro, F. Sanfilippo and A. Todaro, arXiv:1807.07954



UV corrections still significant, leads to a continuum extrapolation with large uncertainties

Continuum value at $T = 430$ MeV in agreement with S. Borsanyi *et al.*, arXiv:1606.07494, where however exact zero modes were forced by hand

How to make the approach to the continuum limit smoother?

Maybe resort to a fermionic definition of topological charge? (work in progress ...)

Concluding remarks

– Nowadays, lattice simulations provide an accurate and reliable numerical tool to study θ-dependence in QCD and QCD-like theories and compare it to various model and phenomenological predictions and approximation schemes;

– Progress is on the way for the study in QCD with light fermions.

Future goals:

$*$ first determination of θ^4 corrections to $f(\theta)$, i.e. b_2, at $T = 0$

$*$ reduction of the impact of UV corrections at high T, improved estimates for axion cosmology