Topological properties of QCD:
from vacuum structure to axion phenomenology

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QCD and θ-dependence

Gauge field configurations relevant to the QCD path integral divide in homotopy classes, characterized by a winding number $Q = \int d^4x\; q(x)$ (Homotopy group $= \mathbb{Z}$)

$$q(x) = \frac{g^2}{64\pi^2} G^a_{\mu\nu}(x) \tilde{G}^a_{\mu\nu}(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} G^a_{\mu\nu}(x) G^a_{\rho\sigma}(x) \qquad G\tilde{G} \propto \vec{E}^a \cdot \vec{B}^a \;\; \text{CPodd quantity}$$

The standard QCD action

$$S_{QCD} = \int d^4x\, \mathcal{L}_{QCD} = \int d^4x \left(\sum_f \bar{\psi}_f \left(D_\mu \gamma_\mu + m_f\right) \psi_f + \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} \right)$$

can be modified by introducing a θ-parameter coupled to Q:

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

$P(Q)$ **is the probability distribution of Q at $\theta = 0$**

The theory at $\theta \neq 0$ is renormalizable and presents explicit CP-breaking

The euclidean path integral measure is complex (sign problem for numerical simulations)

The free energy density $F(\theta) = -T\log Z/V$ is a periodic even function of θ, $F(\theta) \geq F(0)$, which can be expanded and computed around $\theta = 0$ (assuming analyticity)

$$F(\theta) - F(0) = \frac{1}{2}F^{(2)}\theta^2 + \frac{1}{4!}F^{(4)}\theta^4 + \ldots \quad ; \qquad F^{(2n)} = \left.\frac{d^{2n}F}{d\theta^{2n}}\right|_{\theta=0} = -(-1)^n \frac{\langle Q^{2n}\rangle_c}{V_4}$$

$V_4 = V/T$ **is the 4D volume. A common parametrization is:**

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

$$\chi = \frac{1}{V_4}\langle Q^2\rangle_0 = F^{(2)} \qquad b_2 = -\frac{\langle Q^4\rangle_0 - 3\langle Q^2\rangle_0^2}{12\langle Q^2\rangle_0} \qquad b_4 = \frac{\langle Q^6\rangle_0 - 15\langle Q^2\rangle_0\langle Q^4\rangle_0 + 30\langle Q^2\rangle_0^3}{360\langle Q^2\rangle_0}$$

The probability distribution $P(Q)$ of the different topological sectors is not known: it is a non-perturbative property of QCD

Coefficients b_{2n} parametrize deviations of $P(Q)$ from a Gaussian distribution.

The role of fermion fields

An axial $U(1)_A$ rotation of the fermion fields move θ from the gluon to the quark sector (same concept as for the axial anomaly). For any flavor:

$$\psi_f \to e^{i\alpha\gamma_5}\psi_f \qquad \text{and} \qquad \bar{\psi}_f \to \bar{\psi}_f e^{i\alpha\gamma_5}$$
$$\Longrightarrow \quad \theta \to \theta - 2\alpha \qquad \text{and} \qquad m_f \to m_f e^{2i\alpha}$$

- should any quark be massless (this is not the case), θ could be rotated away and θ-dependence would be trivial

- in the presence of light quarks (this is the case), θ-dependence can be reliably studied within the framework of chiral perturbation theory (χPT)

Experimental bounds on the electric dipole of the moment set stringent limits to the amount of CP-violation in strong interactions

$$|\theta| \lesssim 10^{-10}$$

So: why do we bother about θ-dependence at all?

- θ-dependence $\longleftrightarrow P(Q)$ at $\theta = 0$ $\Longrightarrow$ it enters phenomenology anyway.
  e.g., Witten-Veneziano mechanism: $\chi^{YM} = f_\pi^2 m_{\eta'}^2/(2N_f)$

- θ-dependence is a probe of the gauge configurations relevant to the QCD path integral in the different phases of strong interactions

- Strong CP-problem: why is $\theta = 0$? $m_f = 0$ is ruled out.
  A possible mechanism (Peccei-Quinn) invokes the existence of a new scalar field (axion) whose properties are largely fixed by θ-dependence

- Axions are also popular dark matter candidates

Predictions about θ-dependence - I

Dilute Instanton Gas Approximation (DIGA) for high T (Gross, Pisarski, Yaffe 1981)

One can integrate quantum fluctuations around classical solutions with non-trivial winding around the gauge group: instantons. Effective action known only perturbatively. The 1-loop one-instanton contribution is

$$\exp\left(-\frac{8\pi^2}{g^2(\rho)}\right)$$

where $g(\rho)$ is the running coupling at the instanton radius scale ρ.

- by asymptotic freedom, works well for small instantons, which are then exponentially suppressed, implying the validity of a dilute instanton gas approximation (DIGA)

- however, perturbation theory breaks down for large instantons ($1/\rho \lesssim \Lambda_{QCD}$), which become dominant, overlap with each other, and break DIGA

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

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

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

- **At finite T: Instantons of size $\rho \gg 1/T$ suppressed by thermal fluctuations, for high T instantons of effective perturbative action $8\pi/g^2(T)$ dominate. Including also leading order suppression due to light fermions and zero modes:**

$$\chi(T) \sim T^4 \left(\frac{m}{T}\right)^{N_f} e^{-8\pi^2/g^2(T)} \sim m^{N_f} T^{4-\frac{11}{3}N_c - \frac{1}{3}N_f} \propto T^{-7.66} \quad (\text{for } N_f = 2)$$

Notice: perturbative limit implies diluteness, hence DIGA, however DIGA might be good before reaching the asymptotic perturbative behavior

Predictions about θ-dependence - II

Chiral Perturbation Theory (χPT) for low T

At low T, perturbation theory breaks down, however, by $U(1)$ axial rotations, θ can be moved to the light quark masses. Then, χPT can be applied as usual.

Result for the ground state energy (Di Vecchia, Veneziano 1980)

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

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

Explicitly

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

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

Predictions about θ-dependence - III

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

$$L_{QCD}(\theta) = \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} + \theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} G^a_{\mu\nu} G^a_{\rho\sigma}$$

$g^2 N_c = \lambda$ **is kept fixed as** $N_c \to \infty$ $\Longrightarrow$ **if any non-trivial dependence on** θ **exist in the large-**N_c **limit, the dependence must be on** $\bar{\theta} = \theta / N_c$**.**

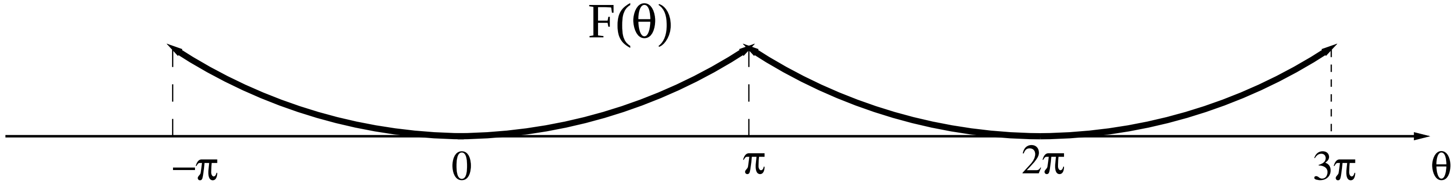
$$F(\theta, T) - F(0, T) = N_c^2 \bar{F}(\bar{\theta}, T)$$

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

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

$$\chi \sim N_c^0 \;\; ; \quad b_2 \sim N_c^{-2} \;\; ; \quad b_{2n} \sim N_c^{-2n}$$

$P(Q)$ **is Gaussian in the large** N_c**. Periodicity in** θ **enforces a multibranched structure with phase transitions at** $\theta = (2k+1)\pi$**.**



Numerical Results from Lattice QCD

main technical and numerical issues

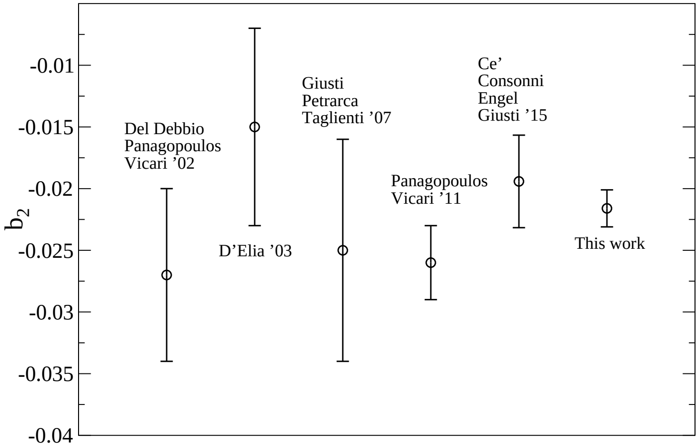
- topological charge renormalizes, naive lattice discretizations are non-integer valued. Various methods devised leading to consistent results
  - field theoretic compute renormalization constants and subtract
  - fermionic definitions use the index theorem to deduce Q from fermionic zero modes
  - smoothing methods use various techniques to smooth gauge fields and recover an integer valued Q (cooling, Wilson flow, smearing ...all substantially equivalent (see e.g. Panagopoulos, Vicari 0803.1593, Bonati, D'Elia 1401.2441, Alexandrou, Athenodorou, Jansen, 1509.04259)

- Determination of higher cumulants is numerically challenging: need to detect deviations from a Gaussian, but as $V_4 \to \infty$ Gaussian modes dominate.

- Freezing of topological modes in the continuum:
  configurations with different Q related by discontinuous field transformations;
  tunneling probability by standard local algorithms decreases exponentially as the continuum limit is approached

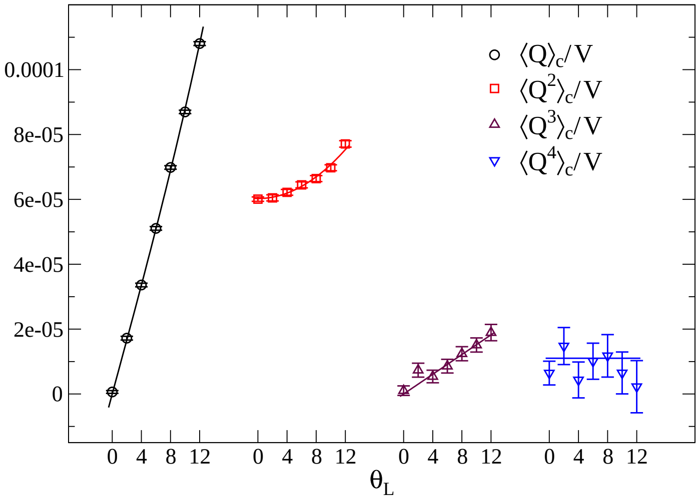
Pure gauge results: $T = 0$

Topological susceptibility well known, with increasing refinement, since 20 years, 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, D'Elia, Scapellato, 1512.01544) obtained by introducing an external imaginary θ source to improve signal/noise.

Introduce an imaginary $\theta = i\theta_L$ in the lattice action, then perform a global fit to the first four cumulants:

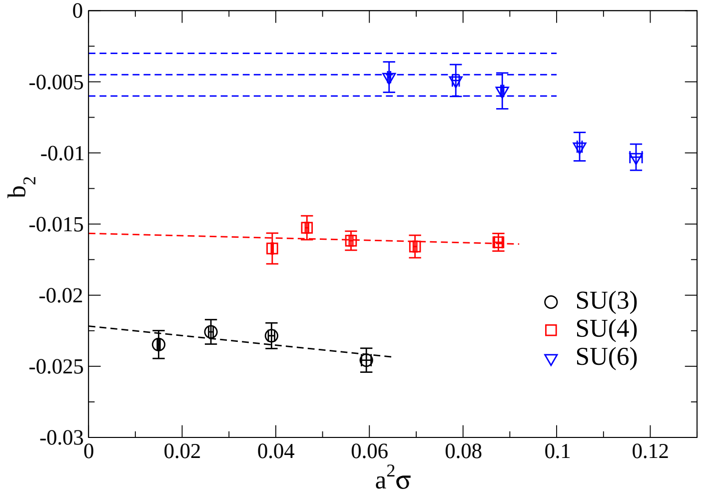


$$\frac{\langle Q \rangle}{\mathcal{V}} = \chi Z \theta_L (1 - 2 b_2 Z^2 \theta_L^2 + 3 b_4 Z^4 \theta_L^4 + \dots)\,,$$

$$\frac{\langle Q^2 \rangle_c}{\mathcal{V}} = \chi (1 - 6 b_2 Z^2 \theta_L^2 + 15 b_4 Z^4 \theta_L^4 + \dots)\,,$$

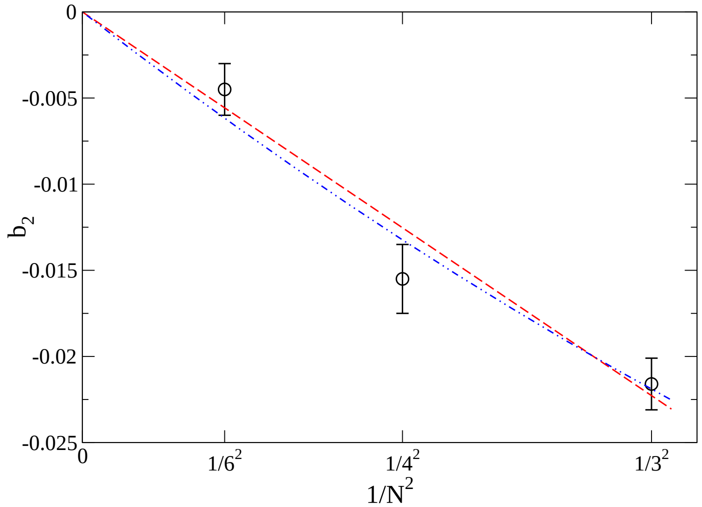
$$\frac{\langle Q^3 \rangle_c}{\mathcal{V}} = \chi (-12 b_2 Z \theta_L + 60 b_4 Z^3 \theta_L^3 + \dots)\,,$$

$$\frac{\langle Q^4 \rangle_c}{\mathcal{V}} = \chi (-12 b_2 + 180 b_4 Z^2 \theta_L^2 + \dots)\,.$$



By these means, we have recently been able to determine the scaling of b_2 to the large N limit.

(Bonati, D'Elia, Rossi, Vicari, 1607.06360)



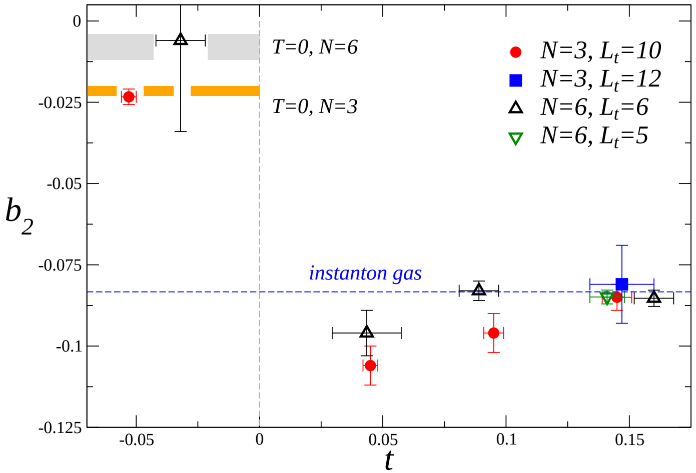
Clear evidence for the predicted large-N_c scaling of b_2:

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

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

Pure gauge results: Finite T, across and above T_c

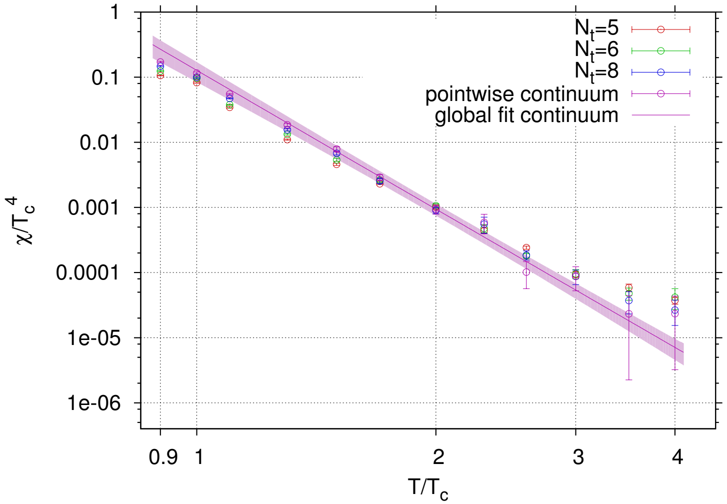
Topological activity stays almost unchanged till T_c and then χ drops suddenly: known since 20 years, but we had some recent progress:



from Bonati, D'Elia, Panagopoulos, Vicari 1301.7640

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

Small deviations compatible with repulsive instanton-instanton interactions



from S. Borsanyi et al. 1508.06917

The perturbative power law behavior predicted for χ at high T has been verified

$\chi(T) \propto 1/T^b$, where $b = 7.1(4)(2)$ (perturbative prediction $b = 7$), but absolute value a factor 10 larger

Emerging picture:

- shortly after T_c, topological excitations behave as a dilute non-interacting gas, $F(\theta) \propto (1 - \cos(\theta))$. Residual interactions around T_c are repulsive. Agreement with perturbative DIGA, at least for the power law.

- the scenario changes completely crossing the confinement transition, large N predictions sets in and $F = F(\theta/N)$.

- Sometimes this is interpreted in terms of decomposition into topological objects with charge $1/N$ (instanton quarks). However our results show that the picture could be naïve, or at least such objects are not weakly interacting.

  Non interacting gas of $1/N$ charged objects would give

$$F \propto (1 - \cos(\theta/N)) \implies b_2 = -\frac{0.08333}{N^2}$$

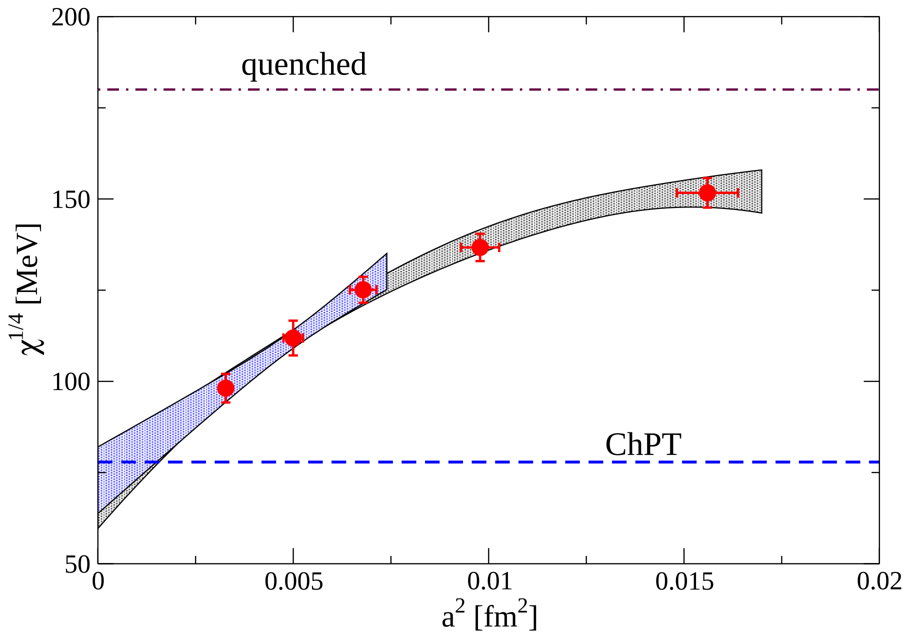
  we obtain instead $b_2 = -0.20(2)/N^2$, hence corrections must be significant.

Full QCD results

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

JHEP 1603 (2016) 155 [arXiv:1512.06746]

We have performed simulations of $N_f = 2 + 1$ QCD, with stout improved staggered fermions, a tree-level Symanzik gauge action, at the physical point (physical quark masses)

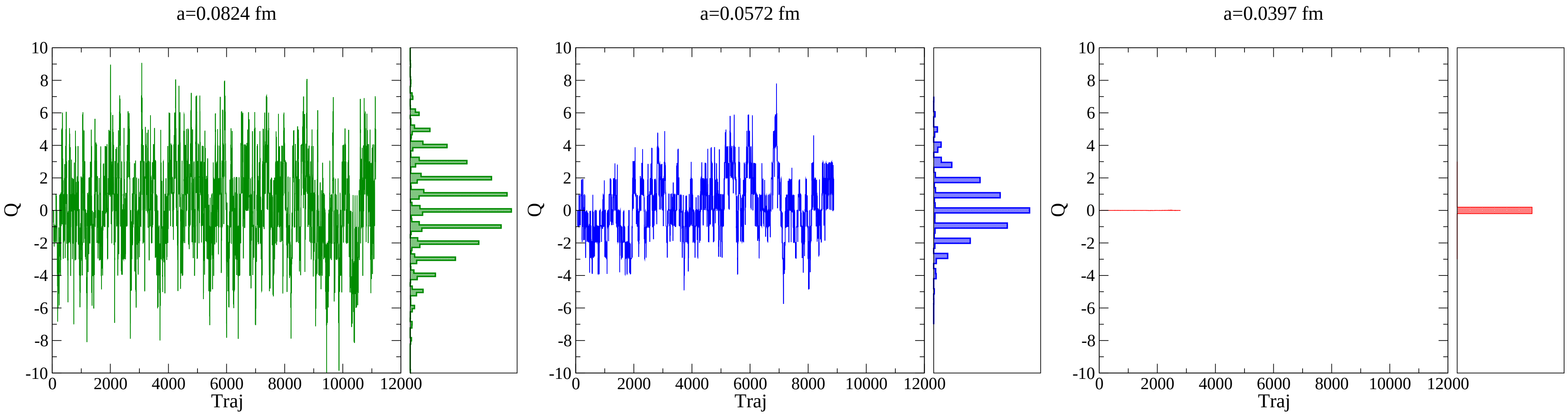


The approach to the continuum limit is quite slow and lattice spacing well below 0.1 fm are needed

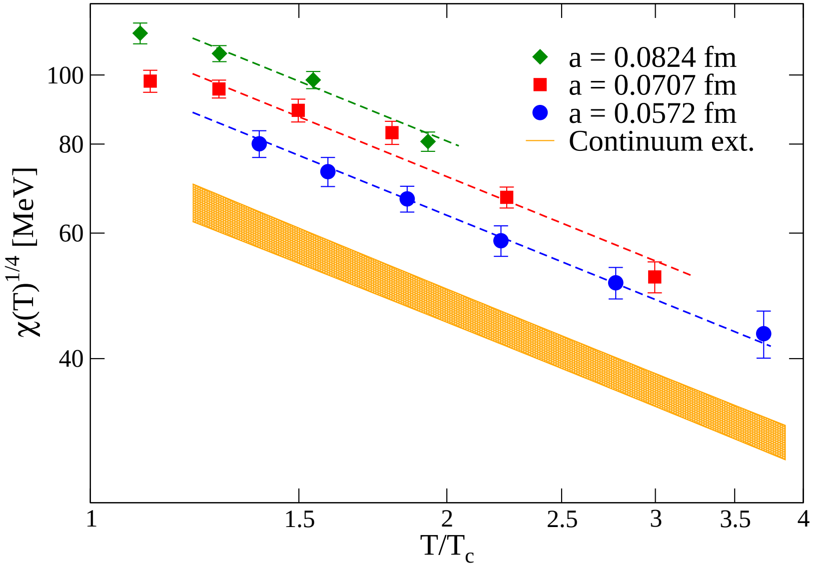
continuum limit compatible with ChPT ($73(9)\mathrm{MeV}$ against $77.8(4)\mathrm{MeV}$)

slow convergence to the continuum is strictly related to the slow approach to the correct chiral properties of fermion fields

The need for quite small lattice spacings, in order to correctly extrapolate to the continuum limit, has brought us to the frontier of frozen topology



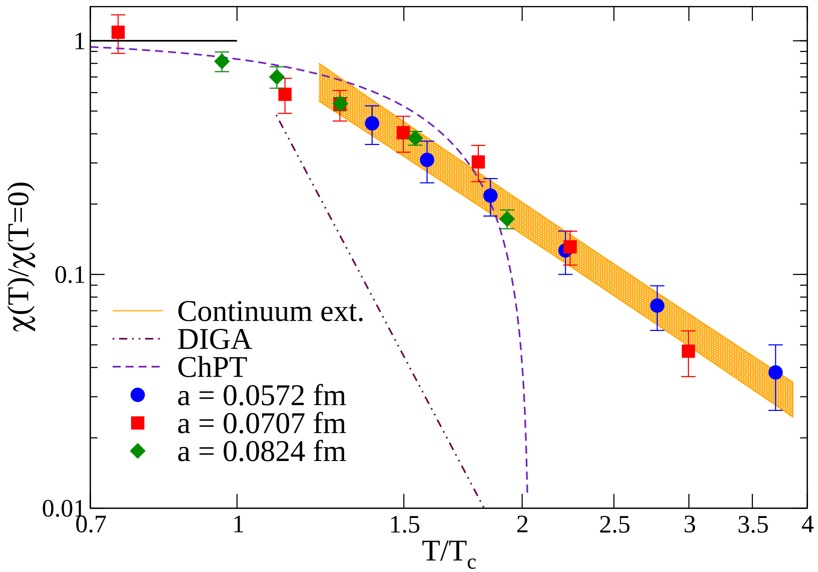
Finite T results provide some surprises



Continuum limit performed according to the following ansatz

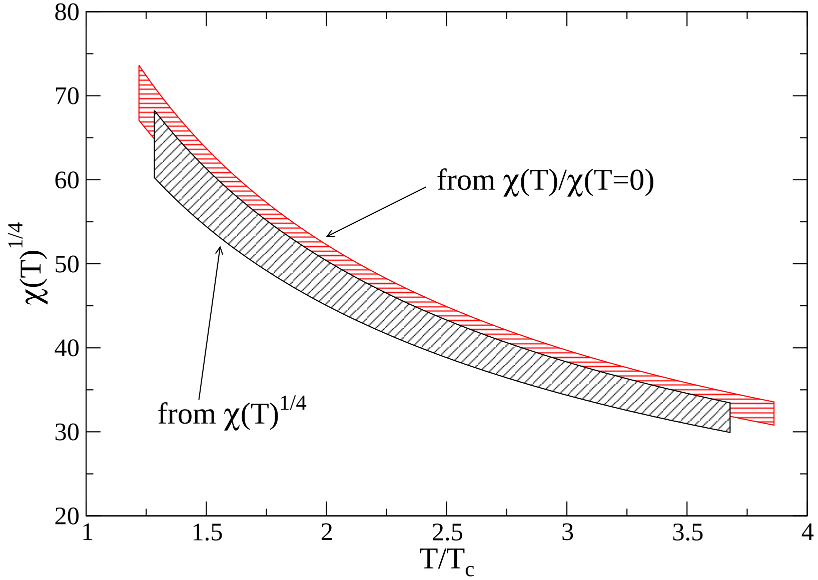
$$\chi^{1/4}(a,T) = A_0(1 + A_1 a^2)\left(\frac{T}{T_c}\right)^{A_2},$$

reliable for $T \lesssim 2\,T_c$ where we have data from three different lattice spacings



Cut-off effects strongly reduced in the ratio $\chi(T)/\chi(T=0)$

drop of the chiral susceptibility much smoother than perturbative estimate: $\chi(T) \propto 1/T^b$ with $b = 2.90(65)$ (DIGA prediction: $b = 7.66 \div 8$)



The two different ways of performing the continuum limit yields perfectly consistent results

How can these results be used to obtain information about axion cosmology?

Consequences for axion physics-I: the QCD axion

Main idea: **add a new scalar field a, with only derivative terms acquiring a VEV $\langle a \rangle$ and coupling to the topological charge density. Low energy effective lagrangian:**

$$\mathcal{L}_{eff} = \mathcal{L}_{QCD} + \frac{1}{2}\partial_\mu a \partial^\mu a + \left(\theta + \frac{a(x)}{f_a}\right)\frac{g^2}{32\pi^2} G\tilde{G} + \ldots$$

- **a is the Goldstone boson of a spontaneously broken (Peccei-Quinn) $U(1)$ axial symmetry (various high energy models exist)**
- **coupling to $G\tilde{G}$ involves the decay constant f_a, supposed to be very large**
- **shifting $\langle a \rangle$ shifts θ by $\langle a \rangle / f_a$. However θ-dependence of QCD breaks global shift symmetry on $\theta_{eff} = \theta + \langle a \rangle / f_a$, and the system selects $\langle a \rangle$ so that $\theta_{eff} = 0$.**
- **Assuming f_a very large, a is quasi-static and its effective couplings (mass, interaction terms) are fixed by QCD θ-dependence. For instance**

$$m_a^2(T) = \frac{\chi(T)}{f_a^2} = \frac{\langle Q^2 \rangle_{T,\theta=0}}{V_4 f_a^2}$$

knowing $F(\theta, T)$ fixes axion parameters during the Universe evolution

Consequences for axion physics-II: misalignment mechanism

Main source of axion relics: misalignment. Field not at the minimum after PQ symmetry breaking. Further evolution (zero mode approximation, $H =$ Hubble constant):

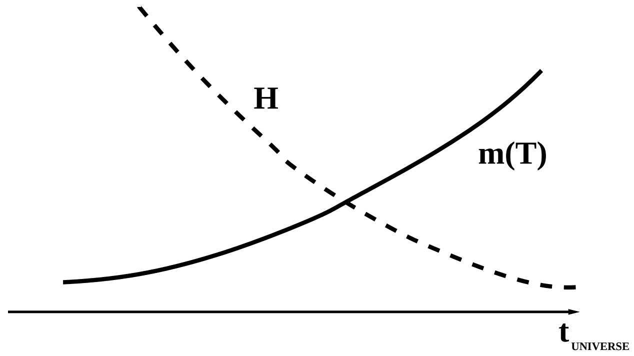
$$\ddot{a}(t) + 3H(t)\dot{a}(t) + m_a^2(T)a(t) = 0 \ ; \quad m_a^2 = \chi(T)/f_a^2$$

$T \gg \Lambda_{QCD}$ 2nd term dominates $\implies \quad a(t) \sim \text{const}$

$m_a \gtrsim H$ oscillations start $\implies$ adiabatic invariant

$N_a = m_a A^2 R^3 \sim$ number of axions ($\sim$ cold DM)

$A =$ oscill. amplitude; $R =$ Universe radius



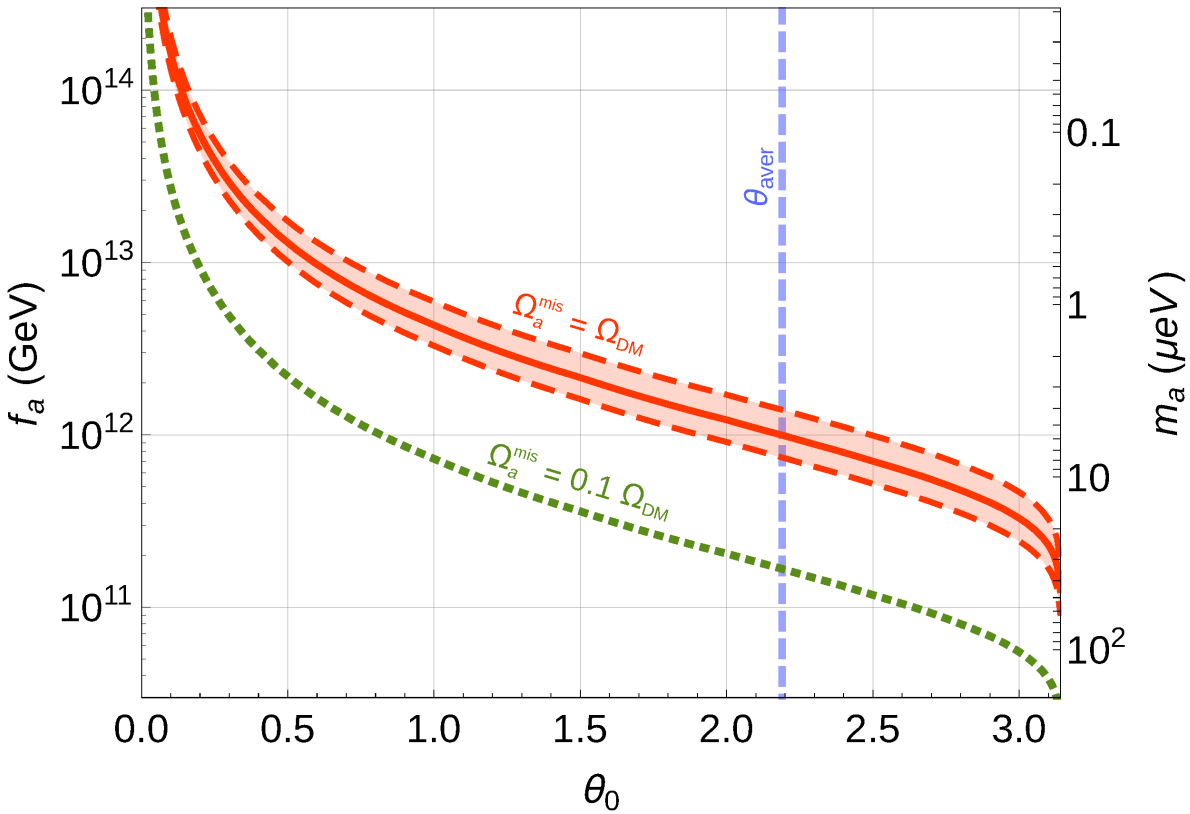
A larger $\chi(T)$ implies larger m_a and moves the oscillation time earlier (higher T, smaller Universe radius R)

Requiring a fixed N_a ($\Omega_{axion} \sim \Omega_{DM}$)

$\chi(T)$ grows $\implies$ oscill. time anticipated $\implies$ less axions $\implies$ require larger f_a to maintain N_a

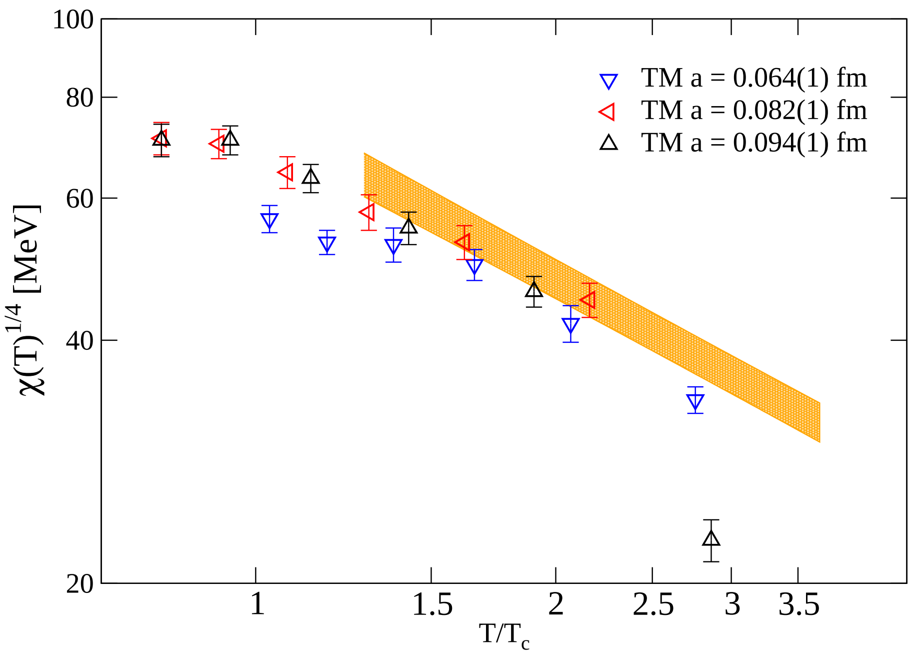
On the other hand, larger f_a means smaller m_a today

Our results translated in predictions for f_a, hence m_a at our times, depending on the required amount of axion dark matter. f_a factor 10 larger (m_a smaller) wrt perturbative DIGA predictions



An unknown variable is the initial misalignment θ_0. Moreover, if PQ symmetry breaks before inflation the initial value is constant, otherwise an average over the initial value has to be performed. order of magnitude prediction for present $m_a \sim 10\ \mu\mathrm{eV}$

Comparison with other determinations

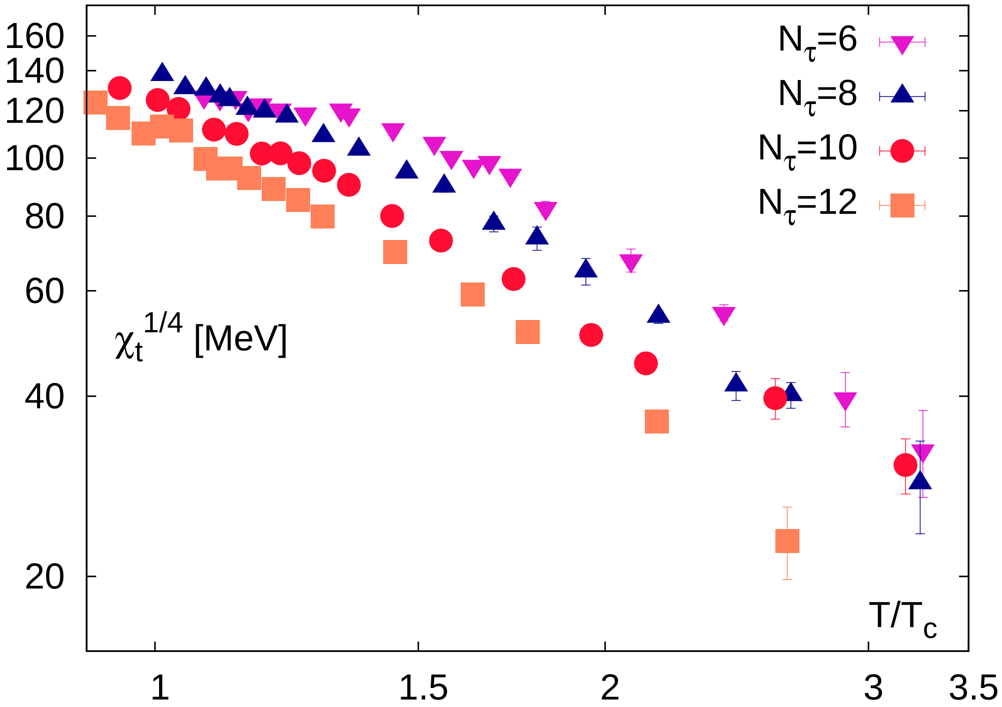


Comparison with results from

A. Trunin, F. Burger, E.-M. Ilgenfritz, M. P. Lombardo, M. Muller-Preussker 1510.02265

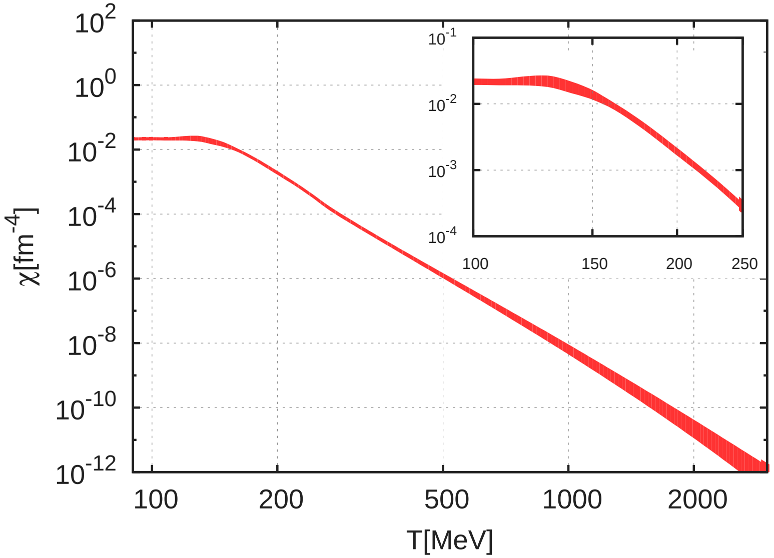
obtained via twisted mass Wilson fermions.

The comparison is made after rescaling according to the DIGA relation $\chi(T) \sim m_q^2 \sim m_\pi^4$ and shows a good agreement with our results.



Results reported in arXiv:1606.0315 (P. Petreczky, H.P. Schadler, S. Sharma).

Numerical simulations with HISQ staggered quarks and almost physical quark masses report a slope more in line with perturbative DIGA expectations for $T \gtrsim 2\,T_c$**.**



A recent approach (Sz. Borsanyi et al, arXiv:1606.07494) permits to reach much higher temperatures and finds agreement with DIGA exponents

main differences:

- the computation of χ at high T is based on the computation of $P(1)/P(0) = Z_{Q=1}(T)/Z_{Q=0}(T)$. That assumes that just the topological sector 1 is relevant, and can be done by simulations at fixed topology (see also J. Frison et al. arXiv:1606.07175)
- gauge configurations with non zero topology are reweighted by appropriate powers of the factor
$$\frac{m}{m + i\lambda}$$
where m is the light quark mass and λ the smallest eigenvalue of the Dirac operator, which should be zero for exact zero modes, to correct for possible lattice artifacts.

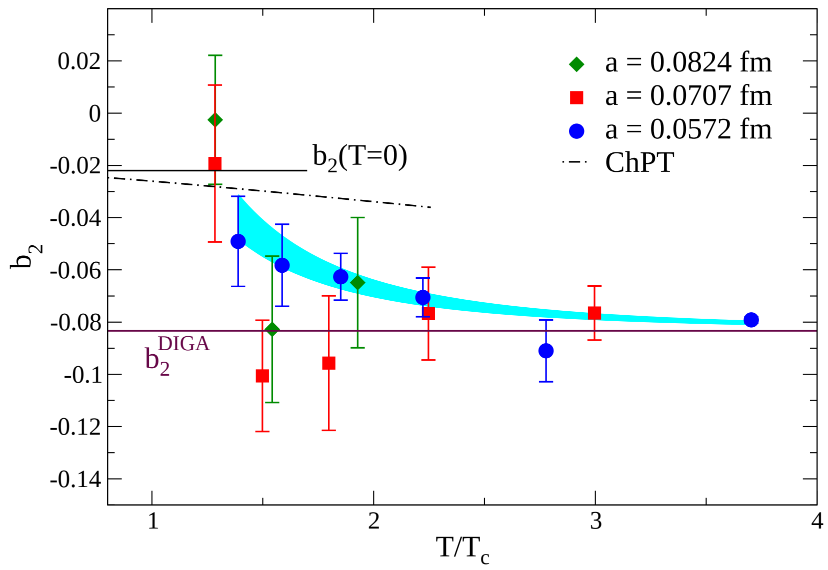
DISCUSSION

Studies reporting results in better agreement with DIGA lead to lower values of f_a, hence higher values of m_a, of the order of $10^2\ \mu\mathrm{eV}$.

The issue is of course very important for experiments trying to detect axions
Therefore the different lattice results should be carefully checked in the future to clarify the origin of possible lattice artefacts and the validity of various assumptions.

A parameter which is sensitive to the validity of the dilute gas approximation is the b_2 coefficient

Our results for b_2



Statistical errors are still large, however deviations from the dilute gas approximation seem detectable till $T \gtrsim 2 - 3\, T_c$.

Morover, deviations seem to be of opposite sign with respect to the quenched case, that could be interpreted in terms of a quark mediated attractive instanton-instanton interactions

The issue deserves further investigations in the future.

Conclusions

- In the quenched case, a clear picture emerges, in which θ-dependence is consistent with a dilute instanton gas for $T > T_c$, and with the large-N expansion for $T < T_c$.

  Future numerical studies should try to increase the precision and obtain information about further b_n coefficients in the confined region

- Our present results on θ dependence in the high T phase of $N_f = 2 + 1$ QCD with physical quark masses contradict the perturbative DIGA prediction, at least for $T \lesssim 600$ MeV, and would shift the axion window by $\sim$ one order of magnitude.

  Other lattice results point in the opposite direction, showing agreement with the perturbative DIGA prediction shortly after T_c.

- The different lattice results should be carefully checked in the future to clarify the origin of possible lattice artefacts and the validity of various assumptions.

  Higher T should be approached by better algorithms, capable of defeating the critical slowing down of topological modes (Resampling methods? Metadynamics? ...)