θ dependence in the deconfined phase of QCD

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Work in collaboration with

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Outline

1. General properties of θ dependence
2. The analytical approaches & the relation with the axions
3. The lattice approach
4. Numerical results
5. Conclusions

The θ parameter

The Euclidean version of the QCD Lagrangian is

$$\mathcal{L}_\theta = \frac{1}{4} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x) - i\theta q(x); \quad q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x)$$

θ is a dimensionless RG-invariant parameter and a nonzero θ value would violate P and CP. Experimentally its value is bounded by $|\theta| \lesssim 10^{-9}$
(Reasons for $\theta = 0$? Strong CP problem)

Nevertheless θ related physics is interesting from various point of view:

- theoretical: the θ dependence is completely nonperturbative
- practical: some features of the hadron spectrum are related to θ (e.g. Witten, Veneziano 1979)
- phenomenologial: e.g. axions to resolve the strong CP problem

The θ dependence of the free energy

Since $F(\theta, T) = F(-\theta, T)$, the free energy can be parametrized as

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

where ($Q = \int q(x)\mathrm{d}x \in \mathbb{Z}$ is the topological charge)

$$\chi = \frac{1}{V_4}\langle Q^2\rangle_{\theta=0}; \qquad b_2 = -\frac{\langle Q^4\rangle_{\theta=0} - 3\langle Q^2\rangle^2_{\theta=0}}{12\langle Q^2\rangle_{\theta=0}}$$

General properties:

- $F(0, T)$ is an absolute minimum of $F(\theta, T)$
- if $\psi_j \to e^{i\alpha\gamma_5}\psi_j$ and $\bar{\psi}_j \to \bar{\psi}_j e^{i\alpha\gamma_5}$ then $\theta \to \theta - 2\alpha N_f$ and $m_j \to m_j e^{2i\alpha}$ (thus $\theta \sim$ complex mass for fermions)
- Q is related to the zero modes of $\not{D}$ with given chirality by the Atiyah-Singer index theorem: $Q = N_R^0 - N_L^0$

Analytical approaches

Large number of colors N (low temperature), Witten 1980

Assume that θ-dependence survives for $N \to \infty$. This requires both $\lambda = g^2 N \to const$ and $\bar{\theta} = \theta/N \to const$ in the large N limit and

$$\chi = \bar{\chi} + o(1); \qquad b_{2n} = \bar{b}_{2n}/N^{2n}\Big(1 + o(1)\Big)$$

Dilute instanton gas (high temperature) Gross, Pisarski, Yaffe 1981

$$b_2 = -\frac{1}{12}; \quad b_4 = \frac{1}{360}; \quad \chi(T) \sim T^4 \left(\frac{m}{T}\right)^{N_f} \exp\big[-S_0\big]$$

From perturbation theory $S_0 = 8\pi^2/g^2(T) \approx (\frac{11}{3}N - \frac{2}{3}N_f)\log(T/\Lambda)$ and

$$\chi(T) \sim m^{N_f}\, T^{4-\frac{11}{3}N-\frac{1}{3}N_f}$$

ChPT (low temperature) Di Vecchia, Veneziano 1980

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

Axion solution of the strong CP problem

Add to SM a pseudoscalar field a with coupling $\frac{a}{f_a}F\tilde{F}$ and only derivative interactions. Since the free energy has a minimum at $\theta = 0$, a will acquire a VEV such that $\theta + \frac{\langle a \rangle}{f_a} = 0$. The simplest possibility is to think of a as the GB of some $U(1)$ axial symmetry (Peccei-Quinn symmetry). The effective low-energy lagrangian is thus

$$\mathcal{L} = \mathcal{L}_{QCD}^{\theta=0} + \frac{1}{2}\partial_\mu a \partial^\mu a + \frac{a(x)}{f_a} q(x) + \frac{1}{f_a}\left(\begin{smallmatrix} model\ dependent \\ terms \end{smallmatrix} \right)$$

Experimental bounds: $f_a \gtrsim 10^9\,\mathrm{GeV}$. We can thus neglect axion loops and use the substitution rule $\theta \to a/f_a$:

$$m_a(T) = \frac{\sqrt{\chi(T)}}{f_a}; \quad m_a(T=0) = \frac{m_\pi f_\pi \sqrt{z}}{(1+z)f_a} \approx 5.70\mu\mathrm{eV}\left(\frac{10^{12}GeV}{f_a}\right)$$

Axions behave as cold dark matter, thus we have the constraint axion density $\leq$ dark matter density. This gives an upper limit for f_a provided we know $f_a(T)$, i.e. during the evolution of the universe.

Topology on the lattice (1)

The topological charge is well defined only for smooth enough gauge configuration, so its definition on the lattice require some care.

Several methods have been devised during the years to study topology on the lattice:

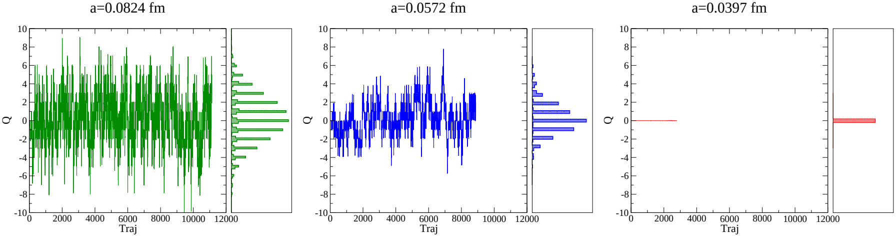
- Field theoretical methods (i.e. take care of finite renormalizations)
- Fermionic methods (overlap fermions)
- Smoothing methods (cooling, smearing, gradient-flow)

All these methods have advantages and drawbacks, nevertheless they have been proven to give compatible results for topological observables (see e.g. Panagopoulos, Vicari 0803.1593, Bonati, D'Elia 1401.2441).

Physical reason: asymptotic freedom (thus relevant distances are $\sim 1/\Lambda \gg a$) and topology (once short distance fluctuations are removed the result is stable "whatever you do").

Topology on the lattice (2)

The topological charge is well defined for smooth enough gauge fields and Monte Carlo updates are almost smooth: as the continuum limit is approached it gets increasingly difficult to correctly sample the different topological sectors ($\sim$ exponential critical slowing down).

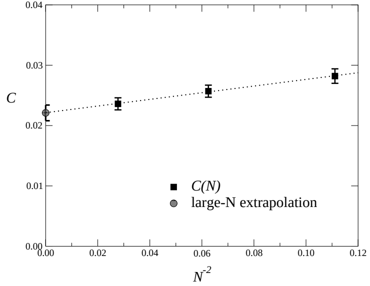


Several algorithmic proposals exist to improve the scaling of autocorrelation times towards the continuum but by now no definitive solution exists. This limit from above the temperatures that can be explored.

$SU(N)$ gauge theory without quarks

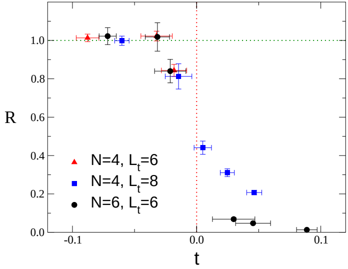
$C = \chi/\sigma^2$, $T = 0$

Del Debbio, Panagopoulos, Vicari 0204125

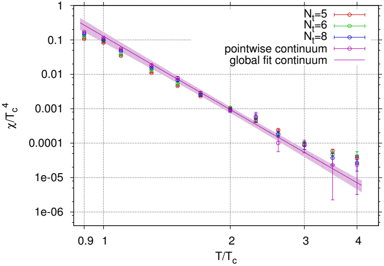


$R = \chi(T)/\chi(T = 0)$

Del Debbio, Panagopoulos, Vicari 0407068

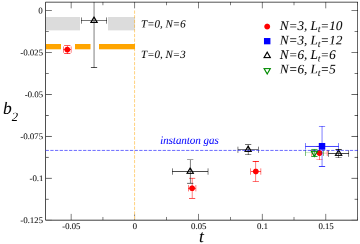


$SU(3)$ S. Borsanyi *et al.* 1508.06917



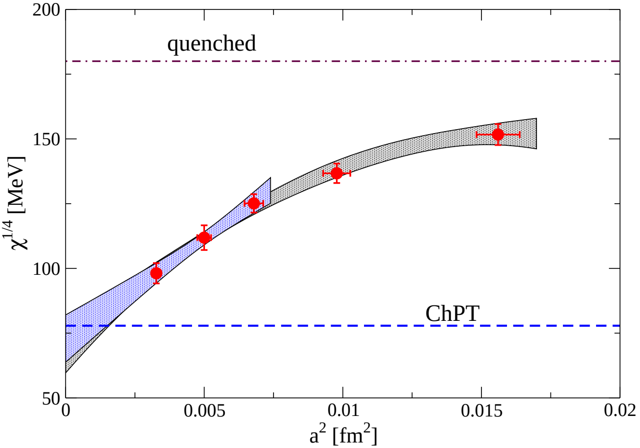
Bonati, D'Elia, Panagopoulos, Vicari 1301.7640

Bonati, D'Elia, Scapellato 1512.01544



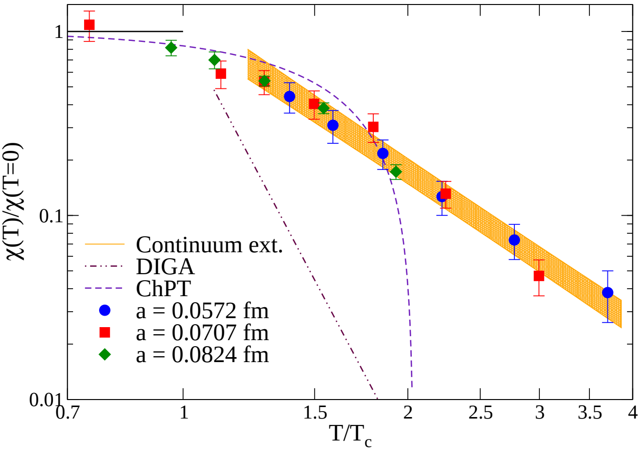
QCD with $2+1$ physical flavours

Check of the method: χ at $T = 0$



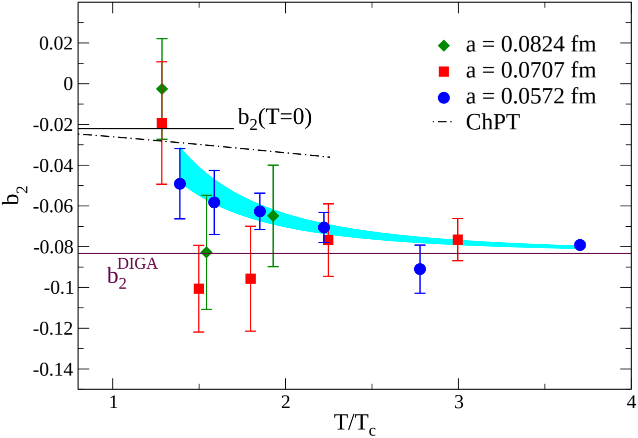
Large cut-off effects but continuum limit compatible with ChPT ($73(9)\mathrm{MeV}$ against $77.8(4)\mathrm{MeV}$)

QCD with $2+1$ physical flavours



Cut-off effect strongly reduced in the ratio $\chi(T)/\chi(T=0)$, moreover $\chi(T) \propto 1/T^b$ with $b = 2.90(65)$ (DIGA prediction: $b = 7.66 \div 8$)

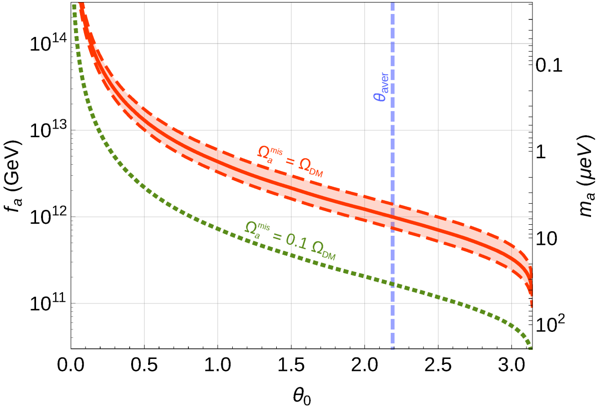
QCD with $2 + 1$ physical flavours



Deviations from DIGA much larger than in pure gauge theories and of opposite sign. Quark mediated instanton interactions?

Axion misalignment contribution to dark matter

Initial condition? If PQ symmetry breaks before inflaction the initial value is constant, otherwise an average on the initial value has to be performed.



Using the DIGA exponent for $\chi(T)$ the upper bound on f_a is underestimated:

$$f_a(\mathrm{DIGA}, \Omega_a^{mis} = \Omega_{DM}) \approx f_a(\mathrm{LQCD}, \Omega_a^{mis} = 0.1\Omega_{DM})$$

Conclusions

We have shown that by using Lattice QCD simulations we can reliably estimate $\chi(T)$ and $b_2(T)$ at the physical point for $T \lesssim 600\,\mathrm{MeV}$.

Several important differences emerges with respect to the case of $SU(N)$ gauge theories without fermions, in particular:

- deviations from DIGA in $b_2(T)$ (which cannot be ascribed to a failure of perturbation theory) are much larger and of opposite sign, i.e. the convergence is from above instead of from below.
- $\chi(T)$ is well described by a behaviour $\sim 1/T^b$ with exponent $b \sim 3$, more than a factor 2 smaller than the commonly adopted DIGA value. This has to be taken into account in computations of the cosmological upper bounds on f_a.

For T large enough we enter the perturbative regime in which DIGA becomes a robust approximation. At which temperature does this happen? It is possible to find lattice evidences of this?

Thank you for your attention!

Backup slides with something more

Large-N argument

$$F^a_{\mu\nu}F^a_{\mu\nu} \text{ and } \epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}F^a_{\rho\sigma} \text{ scale as } N^2$$

To have a nontrivial θ dependence in the large-N limit we have to keep $\bar{\theta} \equiv \theta/N$ fixed, in such a way that θg^2 does not scale with N (fermions are subdominant in the large-N limit).

The large-N scaling form of the free energy is thus (Witten 1980)

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

where $\bar{F}$ is generically nontrivial for $N \to \infty$:

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

By matching the powers of θ we obtain

$$\chi = \bar{\chi} + \cdots$$
$$b_{2n} = \bar{b}_{2n}/N_c^{2n} + \cdots$$

Semiclassical approximation (1)

In general one has (e.g. Coleman "The uses of instantons")

semiclassical approximation $\sim$ weak coupling approximation

Slightly broader perspective:

possibility that a system can be described by means of weakly interacting classical configurations even if the "elementary" coupling is not small

For weakly interacting instantons we have (DIGA, Gross, Pisarski, Yaffe 1981)

$$Z_\theta = \mathrm{Tr} e^{-H_\theta/T} \approx \sum \frac{1}{n_+! n_-!} (V_4 D)^{n_+ + n_-} e^{-S_0(n_+ + n_-) + i\theta(n_+ - n_-)}$$
$$= \exp\left[2 V_4 D e^{-S_0} \cos\theta\right]$$

where $1/D$ is a typical 4−volume. Thus

$$F(\theta, T) - F(0, T) \approx \chi(T)(1 - \cos\theta)$$

Semiclassical approximation (2)

From semiclassical behaviour in the broad sense, using also the leading order suppression due to light fermions and zero modes one gets:

$$b_2 = -\frac{1}{12} \quad b_4 = \frac{1}{360} \quad b_{2n} = (-1)^n \frac{2}{(2n+2)!}$$

$$\chi(T) \sim T^4 \left(\frac{m}{T}\right)^{N_f} \exp\left[-S_0\right]$$

Using also perturbation theory $S_0 = \frac{8\pi^2}{g^2(T)} \approx \left(\frac{11}{3}N - \frac{2}{3}N_f\right)\log(T/\Lambda)$

$$\chi(T) \sim m^{N_f}\, T^{4-\frac{11}{3}N-\frac{1}{3}N_f}$$

(Gross, Pisarski, Yaffe 1981)

Chiral perturbation theory

The θ angle can be eliminated by an $U(1)_A$ rotation at the expense of introducing a complex mass matrix. Chiral perturbation theory can then be applied as usual. The result for the ground state energy is ($T = 0$)

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

(Di Vecchia, Veneziano 1980) thus

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

Explicitly, taking into account also NL effects
Grilli di Cortona, Hardy, Vega, Villadoro 2016

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

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

Axions as dark matter

Cosmological sources of axions: 1) thermal production 2) decay of topological objects 3) misalignment mechanism

Idea of the misalignment mechanism: the EoM of the axion is

$$\ddot{a}(t) + 3H(t)\dot{a}(t) + m_a^2(T)a(t) = 0$$

at $T \gg \Lambda_{QCD}$ the second term dominates and we have $a(t) \sim \mathrm{const}$ (assuming $\dot{a} \ll H$ initially); when $m_a \sim H$ the field start oscillating arount the minimum. When $m_a \gg H$ a WKB-like approx. can be used

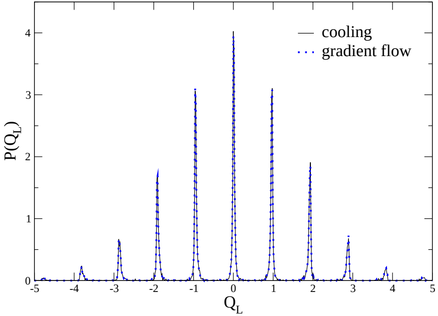
$$a(t) \sim A(t) \cos \int^t m_a(\tilde{t})\mathrm{d}\tilde{t}; \qquad \frac{\mathrm{d}}{\mathrm{d}t}(m_a A^2) = -3H(t)(m_a A^2)$$

and thus the number of axions in the comoving frame $N_a = m_a A^2/R^3$ is conserved.

Overclosure bound: axion density $\leq$ dark matter density

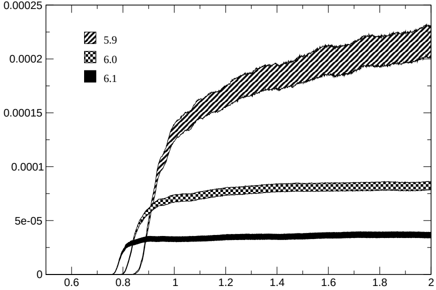
Comparison between smoothing algorithms

Bonati, D'Elia 1401.2441



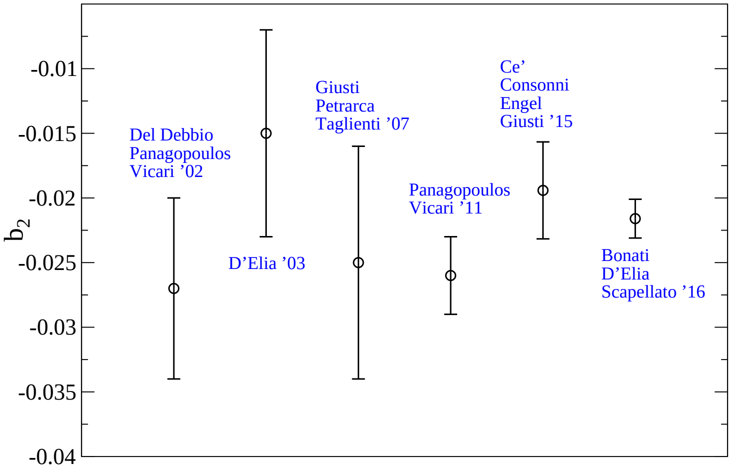
Topological charge distribution obtained by cooling or gradient flow in $SU(3)$ at $\beta = 6.2$.

Del Debbio, Pica 0309145

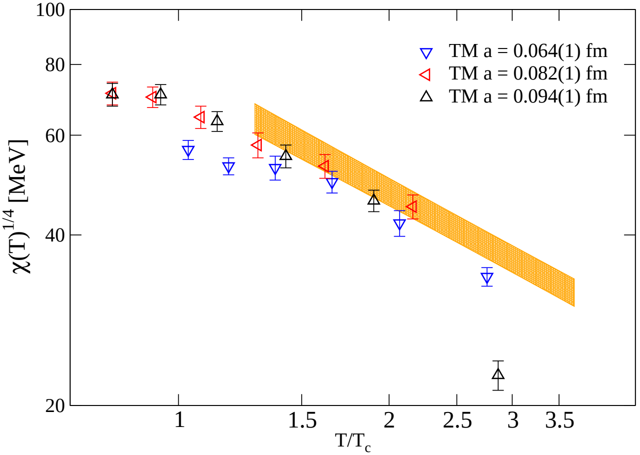


Cooling-like picture displaying the values of the top. susceptibility as a function of the mass used in the overlap Dirac operator in $SU(3)$.

b_2 in $SU(3)$ pure gauge theory



Comparison with $\chi(T)$ from other groups



Comparison with twisted mass data by Trunin et al. 1510.02265 at non-physical quark masses. Data rescaled according to DIGA relation $\chi(T) \propto m_q^2 \propto m_\pi^4$ (and $m_\pi^{TM} \approx 370\,\mathrm{MeV}$) .

Virial-like corrections to DIGA

$F(\theta, T)$ is an even function of period 2π, thus

$$F(\theta, T) - F(0, T) = \sum_{n>0} a_n \left[1 - \cos(n\theta)\right] = \sum_{n>0} c_{2(n-1)} \sin^{2n}(\theta/2)$$

Developing in series we obtain

$$\chi = c_0/2; \quad b_2 = -\frac{1}{12} + \frac{c_2}{8\chi}; \quad b_4 = \frac{1}{360} - \frac{c_2}{48\chi} + \frac{c_4}{32\chi}$$

and c_{2n} contributes only to b_{2m} with $m \geq n$. This is a virial-like expansion and it is reasonable to assume

$$c_{2(n-1)} = d_{2(n-1)} \frac{\chi^n}{\chi^{n-1}(T=0)} \ .$$

The first correction to DIGA is thus

$$F(\theta) = \chi(1 - \cos\theta) + d_2 \frac{\chi^2}{\chi(T=0)} \sin^4(\theta/2)$$

$$b_2 = -\frac{1}{12} + \frac{d_2}{8} \frac{\chi}{\chi(T=0)}, \qquad d_2 = 0.80(16) \ .$$