Topological properties of QCD across deconfinement

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- C. Bonati, M. D'Elia, H. Panagopoulos, E. Vicari Phys. Rev. Lett. **110**, 252003 (2013) [arXiv:1301.7640].
- C. Bonati JHEP **1503** (2015) 006 [arXiv:1501.01172].
- C. Bonati, M. D'Elia, M. Mariti, G. Martinelli, M. Mesiti, F. Negro, F. Sanfilippo, G. Villadoro JHEP **1603** (2016) 155 [arXiv:1512.06746].

Pisa, 7 April 2016

Outline

1. θ dependence: a QM toy model
2. θ dependence: the QCD case
3. Analytic approaches
   - Large N_c
   - Semiclassical methods
   - Chiral perturbation theory
4. Lattice results
   - without light fermions
   - with light fermions
5. PQ symmetry & axions
6. Conclusions

Particle on a circumference (or in a crystal)

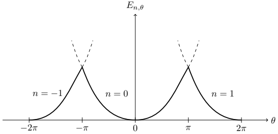
Hamiltonian operator: $H = \frac{1}{2m}p^2 + V(\phi)$ with $V(\phi) = V(\phi + 2\pi)$.
Let R be the 2π rotation operator, then $[H, R] = 0$ and $R^\dagger R = 1$.
Common base of eigenvectors of H and R:

$$H|E,\theta\rangle = E|E,\theta\rangle, \quad R|E,\theta\rangle = e^{i\theta}|E,\theta\rangle, \quad \theta \in [0, 2\pi).$$

The wavefunctions $\psi_{E,\theta}(\phi) = \langle\phi|E,\theta\rangle$ are obtained by solving $H\psi_{E,\theta}(\phi) = E\psi_{E,\theta}(\phi)$ with the b.c. $\psi_{E,\theta}(2\pi) = e^{i\theta}\psi_{E,\theta}(0)$.

In the simple case $V(\phi) \equiv 0$ eigenfunctions and eigenvalues are

$$\psi_{n,\theta}(\phi) = \frac{1}{\sqrt{2\pi}} e^{i(n+\theta/2\pi)\phi}, \quad E_{n,\theta} = \frac{1}{2m}\left(n + \frac{\theta}{2\pi}\right)^2, \quad n \in \mathbb{Z}$$



Note that $\langle\psi_{n,0}|\psi_{m,\theta}\rangle = 0$ *for every* n, m:
θ dependence is nonperturbative!

θ term in the toy model

The usual propagator is given by

$$\langle \phi_f, t_f | \phi_i, t_i \rangle = \sum_k \psi_k(\phi_f)\psi_k^*(\phi_i)e^{-iE_k(t_f - t_i)}$$
$$= \int_{\phi(t_i)=\phi_i}^{\phi(t_f)=\phi_f} [\mathscr{D}\phi] \exp\left(i \int_{t_i}^{t_f} L(\phi)\mathrm{d}t \right)$$

To fix the value of θ in the path-integral approach we can use the identity $\sum_{Q=-\infty}^{+\infty} e^{-iQ(\theta-\theta')} = 2\pi\delta(\theta - \theta')$, thus

$$_\theta\langle \phi_f, t_f | \phi_i, t_i \rangle_\theta = \frac{1}{2\pi} \sum_Q e^{-iQ\theta} \int_{\phi(t_i)=\phi_i}^{\phi(t_f)=\phi_f + 2\pi Q} [\mathscr{D}\phi] \exp\left(i \int_{t_i}^{t_f} L(\phi)\mathrm{d}t \right) =$$
$$= \frac{1}{2\pi} \int_{\phi(t_i)=\phi_i}^{\phi(t_f)=\phi_f} [\mathscr{D}\phi] \exp\left(i \int_{t_i}^{t_f} \left(L(\phi) - \frac{\theta}{2\pi}\dot{\phi} \right) \mathrm{d}t \right)$$

Peculiarities of the θ term $\frac{\theta}{2\pi}\dot{\phi}$

- It is a time derivative (in QCD, a four-divergence): no effect on the equations of motion.
- It explicitly breaks P and T symmetries when $\theta \neq 0, \pi$ (in QCD, possibility of spontaneously broken P, T).
- After Wick rotation

$$\exp\left(i \int L[\phi]\mathrm{d}t - i\theta \int \dot{\phi}\,\mathrm{d}t \right) \to \exp\left(- \int L_E[\phi]\mathrm{d}t - i\theta \int \dot{\phi}\,\mathrm{d}t \right)$$

  thus at $\theta \neq 0$ we can not use Monte-Carlo algorithms (in QCD, P and T can not be spontaneously broken at $\theta = 0$, Vafa-Witten th.).
- θ term exists because of the nontrivial topology of the configuration space: $\pi_1(S^1) = \mathbb{Z}$ (in QCD, because of the nontrivial topology of the gauge group: $\pi_3(SU(N_c)) = \mathbb{Z}$).

Canonical quantizaton of QCD

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu} + \sum_f \bar{\psi}^a_f (i D^{ab}_\mu \gamma_\mu - m_f) \psi^b_f$$

P^a_μ are the conjugate momenta of A^a_μ. The relations between momenta and velocities are $P^a_i = F_{0i}$, $i \in \{1, 2, 3\}$ and $P^a_0 \equiv 0$. The dynamical variables are $A^a_i, P^a_i \equiv -i\hbar\delta/\delta A^a_i$ and the constraint can be written as

$$G^a \equiv \partial_i P^a_i + f^{abc} A^b_i P^c_i = 0$$

Let $\Psi[A]$ be the wave function and $\Delta A^a_i = \partial_i \chi^a - f^{abc} \chi^b A^c_i$ be an infinitesimal gauge transformation. Then

$$\Psi[A + \Delta A] - \Psi[A] \simeq \int \frac{\delta \Psi[A]}{\delta A^a_i} \Delta A^a_i \mathrm{d}x =$$

$$= -\int \left(\chi^a \partial_i \frac{\delta}{\delta A^a_i} + f^{abc} \chi^a A^b_i \frac{\delta}{\delta A^c_i} \right) \Psi[A] \mathrm{d}x \propto \int \chi^a G^a \Psi[A] \mathrm{d}x$$

θ in QCD

The constraint $G^a = 0$ ensures the gauge invariance of the wave function under infinitesimal gauge transformation.
Can every gauge transformation be written as a product of infinitesimal transformations starting from the identity? No! $\pi_3(SU(N_c)) = \mathbb{Z}$.

$$SU(2) \quad \text{example :} \quad \Omega(x) = \exp\left(\frac{i\pi x^a\sigma^a}{\sqrt{x^2+\rho^2}}\right)$$

Let R be the unitary transformation associated to the large gauge transformation Ω. Then

$$H\Psi_{E,\theta}[A] = E\Psi_{E,\theta}[A], \quad R\Psi_{E,\theta}[A] = e^{i\theta}\Psi_{E,\theta}[A], \quad \theta \in [0, 2\pi)$$

The θ term in the lagrangian is

$$\mathcal{L}_\theta = \theta q(x), \quad q(x) \equiv \frac{g^2}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}F^a_{\rho\sigma}, \quad Q = \int q(x)\mathrm{d}x \in \mathbb{Z}$$

General properties of θ dependence

- θ is RG invariant.
- $Z(-\theta, T) = Z(\theta, T)$ ($A \to CP(A)$ in path integral $\sim \theta \to -\theta$)
- Behaviour under $U(1)_A$: 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 $m_j \to m_j e^{2i\alpha}$ (if $m_j = 0$ no θ dependence).
- $F(\theta, T) \geq F(0, T)$:

$$Z(\theta, T) = \int [\mathrm{d}A] e^{-S_E[A] - i\theta Q} = \left| \int [\mathrm{d}A] e^{-S_E[A] - i\theta Q} \right| \leq$$
$$\leq \int [\mathrm{d}A] \left| \cdots \right| = \int [\mathrm{d}A] e^{-S_E[A]} = Z(0, T)$$

- Experimentally θ is compatible with zero ($|\theta| \lesssim 10^{-9}$ from neutron electric dipole moment). Strong CP problem (problem?).
- Most famous example of why θ-dependence matters even if $\theta = 0$: $m^2_{\eta'} = \frac{2N_f}{f_\pi^2}\chi^{N_f=0}$ (Witten-Veneziano formula).

General parametrization of θ dependence

$$F(\theta, T) = -\frac{1}{V_4} \log \int [\mathscr{D}A][\mathscr{D}\bar{\psi}][\mathscr{D}\psi] \exp\left(-\int_0^{1/T} \mathrm{d}t \int \mathrm{d}^3x \, \mathcal{L}_\theta^E \right)$$

$$V_4 = T/V, \quad A_\mu(0, \mathbf{x}) = A_\mu(1/T, \mathbf{x}), \quad \psi(0, \mathbf{x}) = -\psi(1/T, \mathbf{x})$$

General parametrization (assuming analyticity in θ):

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

where

$$\chi = \frac{1}{V_4}\langle Q^2 \rangle_0 \qquad b_2 = -\frac{\langle Q^4 \rangle_0 - 3\langle Q^2 \rangle_0^2}{12\langle Q^2 \rangle_0}$$

$$b_4 = \frac{\langle Q^6 \rangle_0 - 15\langle Q^2 \rangle_0 \langle Q^4 \rangle_0 + 30\langle Q^2 \rangle_0^3}{360\langle Q^2 \rangle_0}$$

Coefficients b_{2n} parametrize deviations of the distribution of topological charge from a Gaussian in the theory at $\theta = 0$.

Large-N_c argument

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

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

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

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

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

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

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 $S_0 = \frac{8\pi^2}{g^2(T)} \approx (\frac{11}{3}N_c - \frac{2}{3}N_f)\log(T/\Lambda)$

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

(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

$$z = 0.48(3) \qquad \chi^{1/4} = 75.5(5)\,\mathrm{MeV} \qquad b_2 = -0.029(2)$$
$$z = 1 \qquad \chi^{1/4} = 77.8(4)\,\mathrm{MeV} \qquad b_2 = -0.022(1)$$

Where to trust the approximations?

Indication that large-N_c can be problematic at $T \neq 0$

By using factorization and translation invariance we get

$$\langle \mathscr{O}(0)\mathscr{O}(Rx)\rangle = \langle \mathscr{O}(0)\rangle\langle \mathscr{O}(Rx)\rangle = \langle \mathscr{O}(0)\rangle\langle \mathscr{O}(x)\rangle = \langle \mathscr{O}(0)\mathscr{O}(x)\rangle$$

thus correlators of scalars are $O(4)$ invariant also at finite temperature.

Indication that instanton calculus can be problematic at $T = 0$

The dominant contributions come from the nonperturbative IR region and some *ad hoc* procedure has to be used to introduce confinement.
For $T > T_c$ no additional confinement length scale is present and T works as an infrared regulator.

Indication that ChPT can be problematic at $T \neq 0$

No chiral symmetry breaking for $T > T_c$.

Topology on the lattice (problem 1)

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

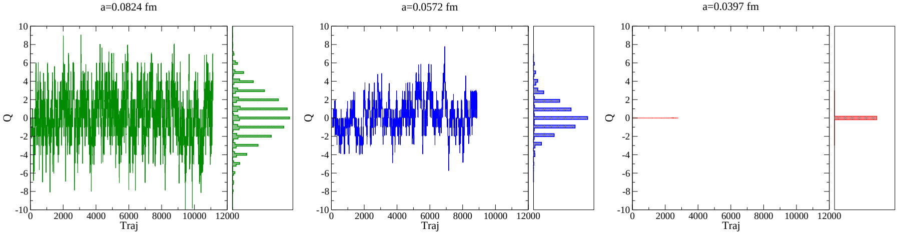
Several methods have been devised during the years to study topology on the lattice:

- Field theoretical methods (perturbative/nonperturbative computation of the renormalization constants)
- Fermionic methods (using the lattice index theorem for Ginsparg-Wilson fermions)
- Smoothing methods

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

Topology on the lattice (problem 2)

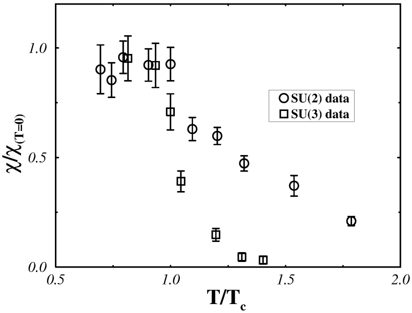
The topological charge is well defined for smooth enough gauge and MC updates are almost smooth: as the continuum limit is approached it gets increasingly difficult to correctly sample the different topological sectors.



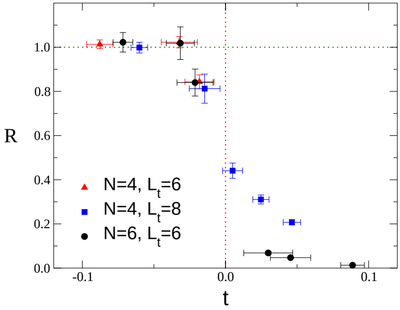
from C. Bonati, M. D'Elia, M. Mariti, G. Martinelli, M. Mesiti, F. Negro, F. Sanfilippo, G. Villadoro 1512.06746.

$SU(N)$ theories across T_c (1)

B. Alles, M. D'Elia, A. Di Giacomo 9706016



L. Del Debbio, H. Panagopoulos, E. Vicari 0407068

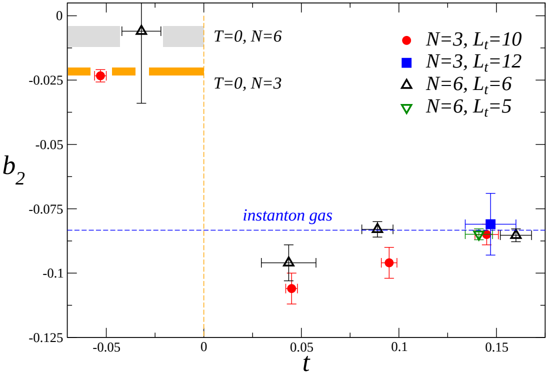


The topological susceptibility is constant for $T \lesssim T_c$ and then abruptly decreases.

$SU(N)$ theories across T_c (2)

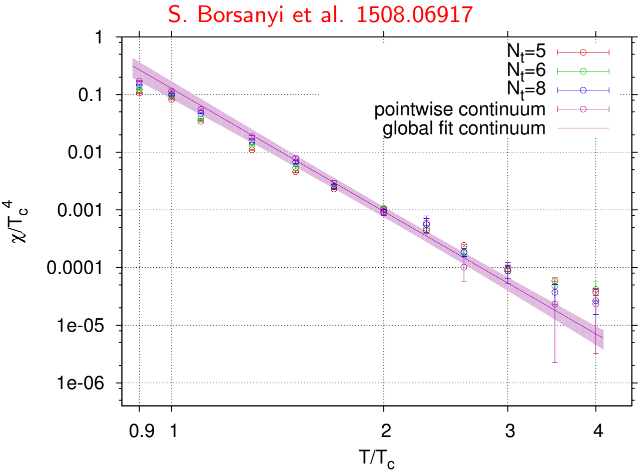
C. Bonati, M. D'Elia, H. Panagopoulos, E. Vicari 1301.7640

(C. Bonati, M. D'Elia, A. Scapellato 1512.01544)



- large-N_c scaling for $T < T_c$, b_2 independent of N_c for $T > T_c$
- DIGA values ($b_2 = -1/12$, $b_4 = 1/360$) reached for $T \gtrsim 1.1 T_c$

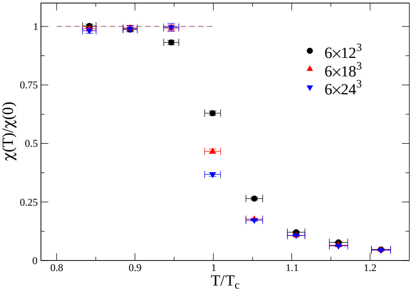
$SU(3)$ theory for $T > T_c$

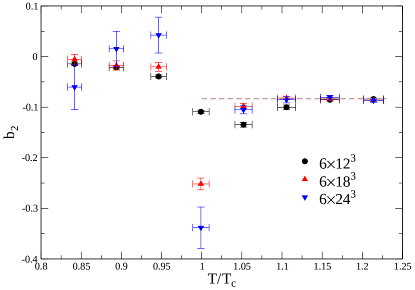


$\chi(T) \propto 1/T^b$, where $b = 7.1(4)(2)$ (DIGA prediction $b = 7$).

G_2 theory across T_c

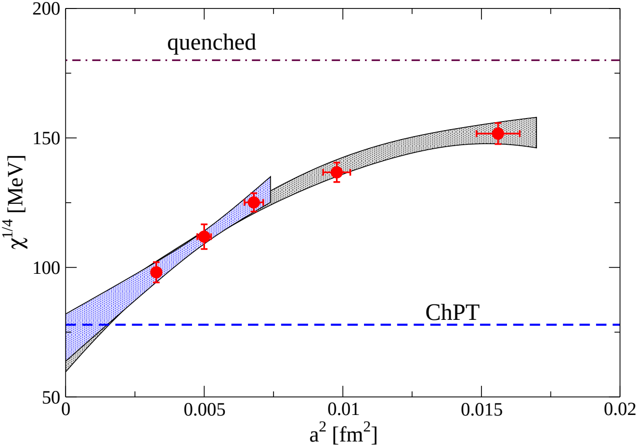
C. Bonati 1501.01172





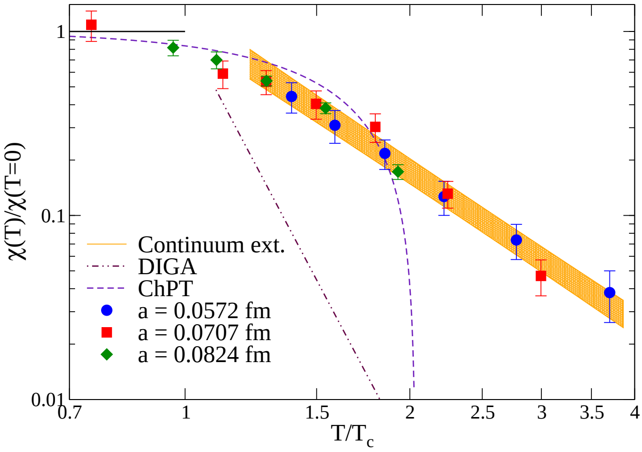
Everything looks the same as in $SU(N)$ theories, but in G_2 no large-N_c limit exists! Alternative explanation? Relation to confinement?

QCD at $T = 0$ (from 1512.06746)



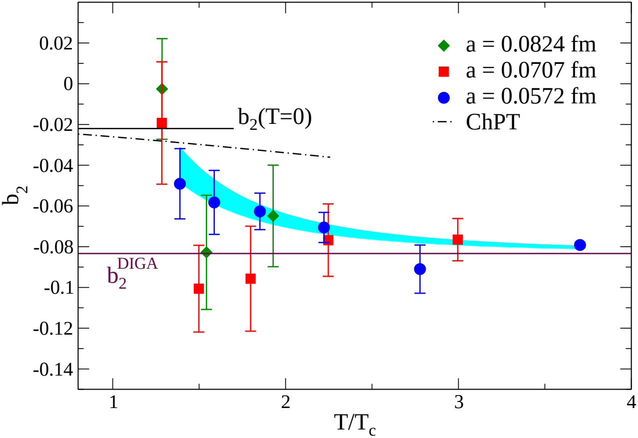
Large cut-off effects but continuum limit compatible with ChPT ($73(9)\mathrm{MeV}$ against $77.8(4)\mathrm{MeV}$)

QCD at $T \gtrsim T_c$ (from 1512.06746)



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 at $T \gtrsim T_c$ (from 1512.06746)



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

Possible solutions of the strong CP problem

1. At least a massless quark ($m_u = 0$).
2. Assume a CP invariant lagrangian for the standard model and explain CP violation by CP SSB.
3. "Dynamical" θ angle.

Realization of mechanism 3: 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 $\theta + \frac{\langle a \rangle}{f_a} = 0$.

Goldstone bosons have only derivatives coupling, so 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

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

Simplest theoretical model (Kim, Shifman, Vainshtein, Zakharov)

Q =new quark, ϕ =new complex scalar

$$\mathcal{L} = \frac{1}{2}|\partial_\mu\phi|^2 + \bar{Q}i\not{D}Q + \lambda\phi\bar{Q}_L Q_R + h.c - V(|\phi|^2)$$

$$U(1)_{PQ} : \begin{cases} \phi \to e^{i\alpha}\phi \\ Q \to e^{-i\frac{\alpha}{2}\gamma_5}Q \end{cases} \qquad \text{After SB } \phi = \frac{v_{PQ}}{\sqrt{2}}e^{ia/v_{PQ}}$$

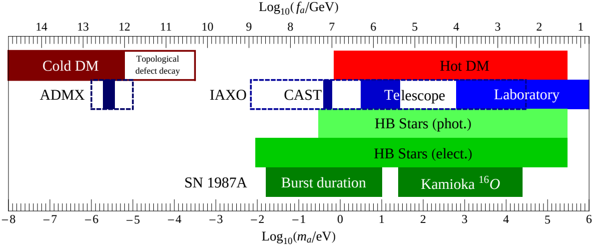
Rotating away the phase we obtain a mass term $\lambda\frac{v_{PQ}}{\sqrt{2}}\bar{Q}Q$ for the new fermion and the coupling of the axion with the gluons $\frac{a}{v_{PQ}}q(x)$.

If we have N_f flavours of Q, then $f_a = v_{PQ}/N_f$ and $U(1)_{PQ} \to Z_{N_f}$. If Q is EM charged we obtain a direct coupling to photons.

(other famous model: Dine, Fischler, Srednicki, Zhitnitskii, Peccei, Quinn, Weinberg, Wilczek)

Axions and QCD vacuum

Cadamuro 1210.3196



The coupling f_a turns out to be very large, so in computing the free energy we can safely neglect axion loops. We can thus use the substitution rule $\theta \to a/f_a$ and the square mass of the axion is related to χ, its fourth coupling to b_2 and so on. Explicitly

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

Axions 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

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

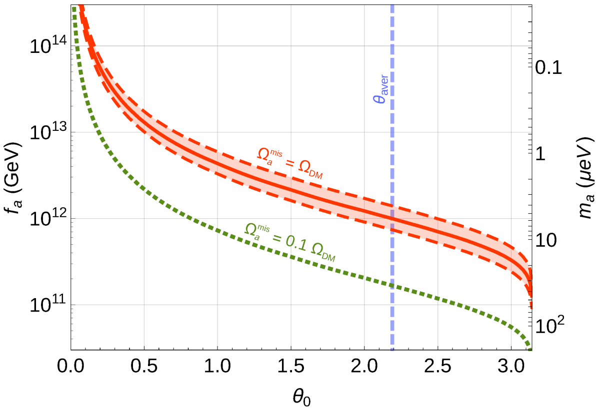
at $T \gg \Lambda_{QCD}$ the second term dominates and we have $a(t) \sim \mathrm{const}$ (assuming $\dot{a} \ll H$ initially); when $m_a \sim H$ the field start oscillating arount the minimum. When $m_a \gg H$ a WKB-like approx. can be used

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

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

Axions as dark matter (from 1512.06746)



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

Conclusions

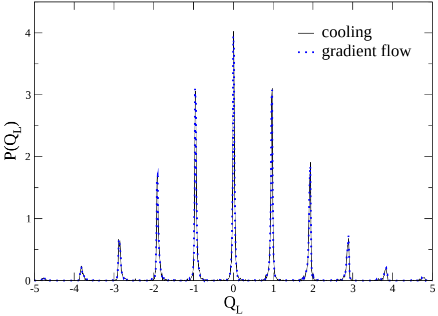
- For $SU(N_c)$ gauge theory without fermions
  - the deconfinement transition can be interpreted as a transition between large-N_c and instanton behaviours for the θ dependence
  - b_{2n} coefficients enter the DIGA regime for $T \gtrsim 1.1 T_c$, deviations indicate repulsive interactions between instantons
  - $\chi(T)$ well described by the DIGA behaviour $\chi(T) \sim T^{-7}$ (Is this accidental?)
- For the G_2 theory without fermions everything goes like for $SU(N_c)$ but no large-N_c limit exists (Indication of a general relation between topology and confinement?)
- For $N_f = 2+1$ QCD
  - the convergence of b_{2n} to the DIGA prediction is slower and deviations indicate attractive insteractions between instantons
  - $\chi(T)$ shows strong deviation from DIGA for $T \lesssim 4 T_c$ (When DIGA sets in? Simulations at higher temperature needed. Algorithms for performing these simulations needed)
  - the limits on f_a from misalignment mechanism increase by almost an order of magnitude

Thank you for your attention!

Backup slides with something more

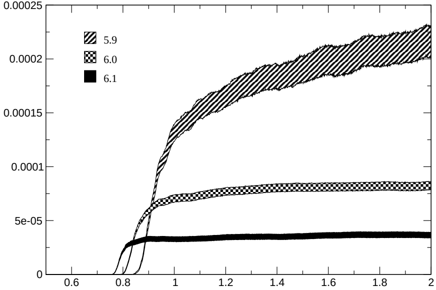
Comparison between smoothing algorithms

Bonati, D'Elia 1401.2441



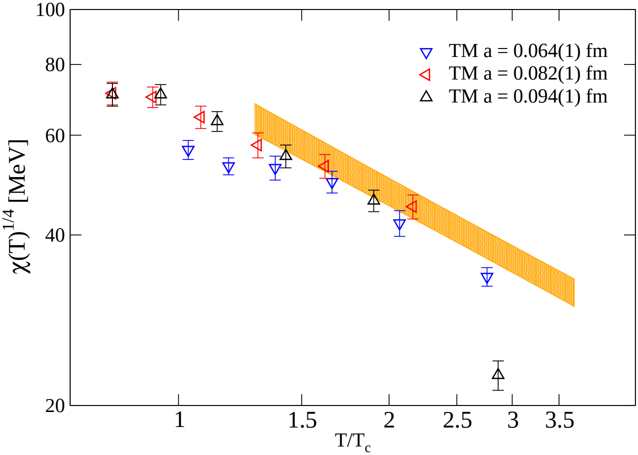
Topological charge distribution obtained by cooling or gradient flow in $SU(3)$ at $\beta = 6.2$.

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 $SU(3)$.

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

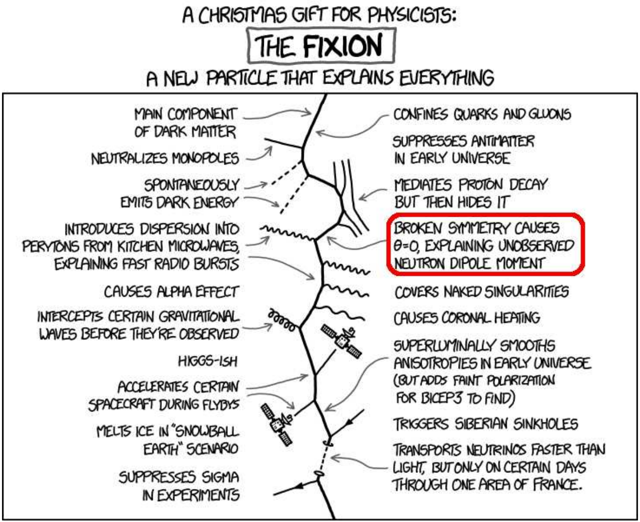
$$c_{2(n-1)} = d_{2(n-1)} \frac{\chi^n}{\chi^{n-1}(T=0)} \, .$$

The first correction to DIGA is thus

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

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

Axions as an "easy solution" of strong CP problem



http://imgs.xkcd.com/comics/fixion.png