θ-dependence of QCD and QCD-like theories

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Neutron Electric Dipole Moment: from theory to experiment - ECT*, 1 August 2022

OUTLINE

- θ-dependence in QCD and available predictions

- θ-dependence from lattice QCD: main technical issues

- Lattice results for $SU(N)$ pure gauge theories:

  how θ-dependence changes across the various phases
  and how the phase diagram itself is influenced by θ

Many non-perturbative properties of strong interactions are related to the presence in the path-integral of configurations with non-trivial topology.

gauge configurations divide into non-trivial homotopy classes, labelled by an integer winding number $Q = \int d^4x \; q(x)$

$$q(x) = \frac{g^2}{32\pi^2} G^a_{\mu\nu}(x) \tilde{G}^a_{\mu\nu}(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} G^a_{\mu\nu}(x) G^a_{\rho\sigma}(x)$$

$$q(x) = \partial_\mu K_\mu \;\; ; \quad K_\mu \equiv \frac{g^2}{16\pi^2} \epsilon_{\mu\nu\rho\sigma} A^a_\nu \left(\partial_\rho A^a_\sigma + \frac{1}{3} g f^{abc} A^b_\rho A^c_\sigma \right)$$

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

$q(x)$ **is a total derivative, but global topology makes it non-trivial**
Homotopy group: $\pi_3(SU(3)) = \mathbb{Z}$ (**actually,** $\pi_3(SU(N)) = \pi_3(SU(2)) \; \forall \; N$)

$G\tilde{G}$ **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.**

Non-trivial θ**-dependence emerges because of the existence of configurations with finite action and** $Q \neq 0$

classical solutions: instantons and anti-instantons

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

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

and to BSM physics too (axion cosmology)

Numerical computations are made difficult by the appearance of a complex factor in the path-integral: sign problem

How to compute QCD at non-zero θ

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

It can be related 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

Dynamical fermions enter the game in a non-trivial way, essentially because of the Atiyah-Singer index theorem and the axial anomaly equation:

$$\textbf{Index theorem} \quad \Longrightarrow \quad Q = D = n_+ - n_- = \textbf{Tr}(\gamma_5)$$

where $n_\pm$ are, respectively, the number of left-handed and right-handed zero-modes of the Dirac operator D.

$$\textbf{Axial anomaly} \quad \Longrightarrow \quad \partial_\mu j^5_\mu = 2N_f q(x) \;\; ; \quad j^5_\mu = \sum_{f=1}^{N_f} \bar{\psi}_f \gamma_\mu \gamma_5 \psi_f$$

An axial $U(1)_A$ rotation on fermion fields moves θ to the quark sector

$$\psi_f \to e^{i\alpha\gamma_5}\psi_f, \;\; \bar{\psi}_f \to \bar{\psi}_f e^{i\alpha\gamma_5} \quad \Longrightarrow \quad \theta \to \theta - 2\alpha \;\; \textbf{and} \;\; m_f \bar{\psi}_f \psi_f \;\; \textbf{gets a complex phase}$$

Interplay with light fermions

- in the presence of massless quarks, θ can be freely changed, $\theta \to \theta - 2\alpha$, with no other effect, hence one expects a trivial θ-dependence

  Intuitive understanding:

$$Z(\theta) = \int \mathcal{D}U e^{-S_{YM}} \det(D + m_f) e^{i\theta Q}$$

  for $m_f = 0$, the determinant vanishes because of the zero modes when $Q \neq 0$

  $\Longrightarrow \quad P(Q) = 0$ for $Q \neq 0$

- in the presence of light quarks, the θ term can be moved to the (small) mass term, hence 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 with θ-dependence at all?

- θ-dependence $\longleftrightarrow P(Q)$ at $\theta = 0$ $\implies$ it enters phenomenology anyway.
  e.g., Witten-Veneziano mechanism:
  $$\chi^{YM}_{large\ N} = \frac{f_\pi^2}{2N_f}\left(m^2_{\eta'} + m^2_{\eta'} - 2m^2_K\right) \implies \chi^{YM}_{large\ N} \simeq (180\ \mathrm{MeV})^4$$
- Rich interplay between θ-dependence and QCD phase structure
- Strong CP-problem: why $\theta = 0$? $\quad m_f = 0$ 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 popular dark matter candidates, so the issue is particularly important
  $\rightarrow$ Claudio Bonanno's talk on Friday

Predictions about θ-dependence - I

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

Can we integrate around classical solutions?

Effective action known only perturbatively. The one-instanton contribution is
$\exp\left(-8\pi^2/g^2(\rho)\right)$ **times a prefactor depending on a 1-loop computation**
$g(\rho)$ **is the running coupling at the instanton 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.**
  Indeed, the instanton size distribution has an IR divergence:

$$dn_I \sim d^4x\, d\rho\, \rho^{11N_c/3-5}$$

DIGA may work well only in the presence of an effective IR cutoff, like, e.g., a finite temperature $T \gtrsim \Lambda_{QCD}$

DIGA prediction for θ-dependence

- **Instantons and Anti-Instantons are treated as uncorrelated (non-interacting) objects**

  $\Longrightarrow$ **Poisson distribution with an average probability density p per unit volume**

$$Z_\theta \propto \sum_{n_-,n_+=0}^{\infty} \frac{1}{n_+!n_-!}(V_4 p)^{n_+ + n_-} e^{i\theta(n_+ - n_-)} = \exp\left[V_4 p(e^{i\theta} - e^{-i\theta})\right] = e^{2V_4 p \cos\theta}$$

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

- **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 leading order contributions from light fermions:**

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

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

Predictions about θ-dependence - II

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

Instanton computation is expected to fail at low T. It would also give a vanishing θ-dependence in the large-N_c limit, contrary to Witten-Veneziano formula.

Indeed, since $g^2 N_c = \lambda$ is kept fixed as $N_c \to \infty$ ('t Hooft scaling):

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

Standard argument by E. Witten (Nucl.Phys.B 156 (1979) 269-283)

$$L_{YM}(\theta) = \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} + \theta \frac{g^2}{32\pi^2} G^a_{\mu\nu} \tilde{G}^a_{\mu\nu} = \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} + \theta \frac{\lambda}{32\pi^2 N_c} G^a_{\mu\nu} \tilde{G}^a_{\mu\nu}$$

the natural variable is θ/N_c, and the vacuum energy, including its θ dependence, must be proportional to N_c^2 (numbers of degrees of freedom)

$$F(\theta) = N_c^2 \bar{F}(\bar{\theta})$$

where $\bar{F}$ has a non-trivial dependence on $\bar{\theta}$ for $N_c \to \infty$

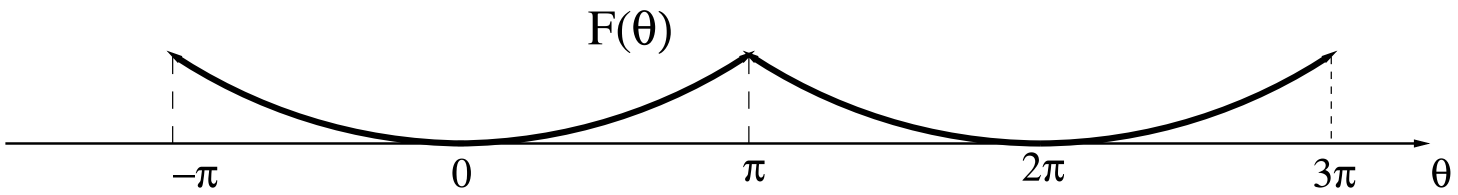
Large-N_c scaling: consequences

$$\Delta F(\theta) = F(\theta) - F(0) = N_c^2 \left(\text{power series in } \bar{\theta}^2\right) = \frac{\chi}{2}\theta^2 \left(1 + b_2\theta^2 + b_4\theta^4 + \dots\right)$$

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 limit. Periodicity in θ enforces a multibranched structure with phase transitions at $\theta = (2k+1)\pi$ (like in the QM model at $T = 0$)



Further observations:

- **Is it like having effective degrees of freedom with fractional $Q \propto 1/N_c$?**
  Maybe, but lattice simulations show they are not weakly interacting
- **Large-N_c predictions are more quantitative for vector-like models**
  e.g., for CP^{N-1} models in two dimensions

Predictions about θ-dependence - III

Chiral Perturbation Theory (χPT) for low T

In the presence of light fermions, θ can be moved to the light quark sector by a $U(1)$ axial rotation. 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

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

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

this is the physical case and fixes the axion mass $\Longrightarrow \quad m_a \sim 10^{-5} \left(\frac{10^{12}\,\mathrm{GeV}}{f_a} \right)$

Studying topology on the lattice

outline of main questions about θ-dependence

- **Check of large-N_c predictions (Witten-Veneziano formula, scaling of b_{2n} coefficients)**

- **Is there a transition to a DIGA regime at high T? Where? Any relation with confinement/deconfinement?**

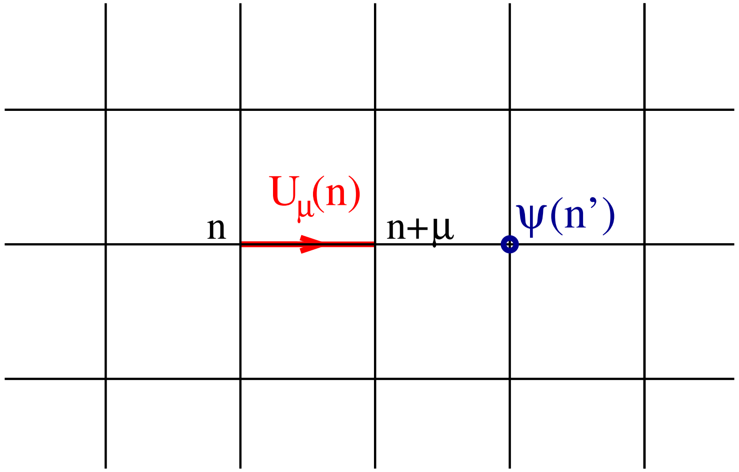
- **How does θ influence the QCD phase diagram?**

- **Useful predictions for axion cosmology?**
  $\rightarrow$ **talk by Claudio Bonanno**

- **Non-perturbative predictions for the electric dipole moment of the neutron?**
  $\rightarrow$ **main topic of this workshop**

Studying topology on the lattice

basic introduction



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, fermion matrix written in terms of gauge fields

$$M[U] = D_\mu \gamma_\mu + m_q$$

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

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

τ is the extension of the compactified time

Studying topology on the lattice

outline of main issues and technical problems

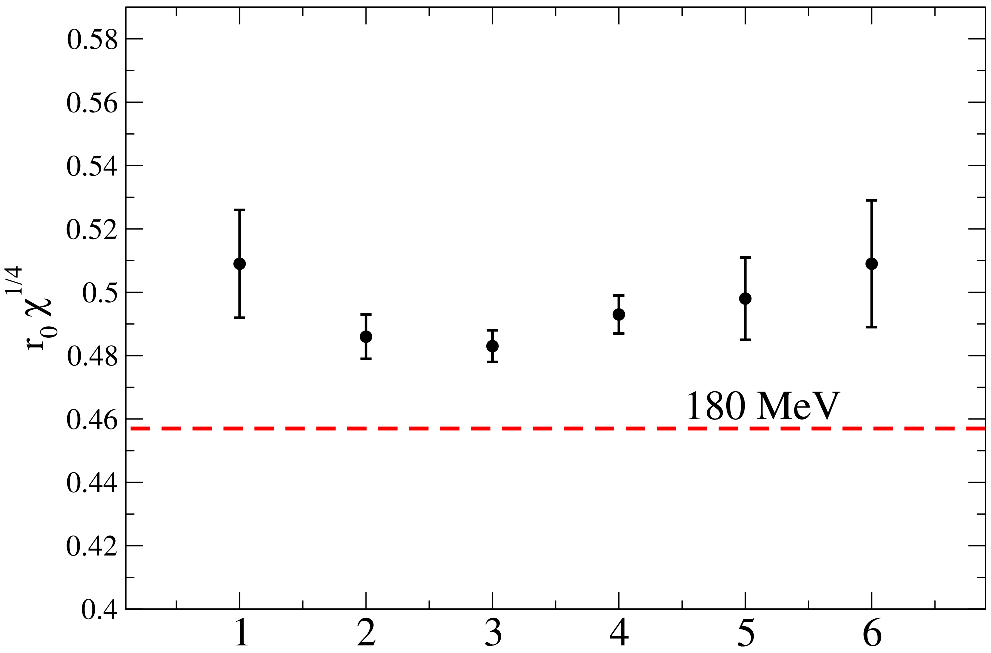
- **Renormalization issues**
  - Choose a discretization of Q (either gluonic or fermionic)
  - Take care of renormalizations or make use of smoothing techniques to suppress them
- **Control on continuum limit extrapolation**
  - approach to continuum limit can be much worse in the presence of light fermions
  - $\det(D+m)$ should suppress $Q \neq 0$, but fails because of bad chiral properties of the discretization
- **Access to higher order cumulants**
  - Discrimination between different predictions for θ-dependence needs access to $O(\theta^4)$ in $F(\theta)$
  - Having access to $\theta = 0$ simulations only, that requires measuring tiny deviations from an almost Gaussian distribution
- **Algorithmic issues: critical slowing down and sampling of rare events**
  - in the continuum limit, homotopy classes are no more connected by finite action configurations. Algorithms may lose ergodicity (problem increases exponentially at large N)
  - in a finite volume, it may happen that $\langle Q^2 \rangle = \chi V \ll 1$. One may need prohibitively long runs to achieve enough statistics

Results from various methods for χ in $SU(3)$ pure gauge - $T = 0$

agreement when expressed in the same units: Sommer parameter $r_0 \simeq 0.5$ fm (r_0/a from R. Sommer, arXiv:1401.3270)

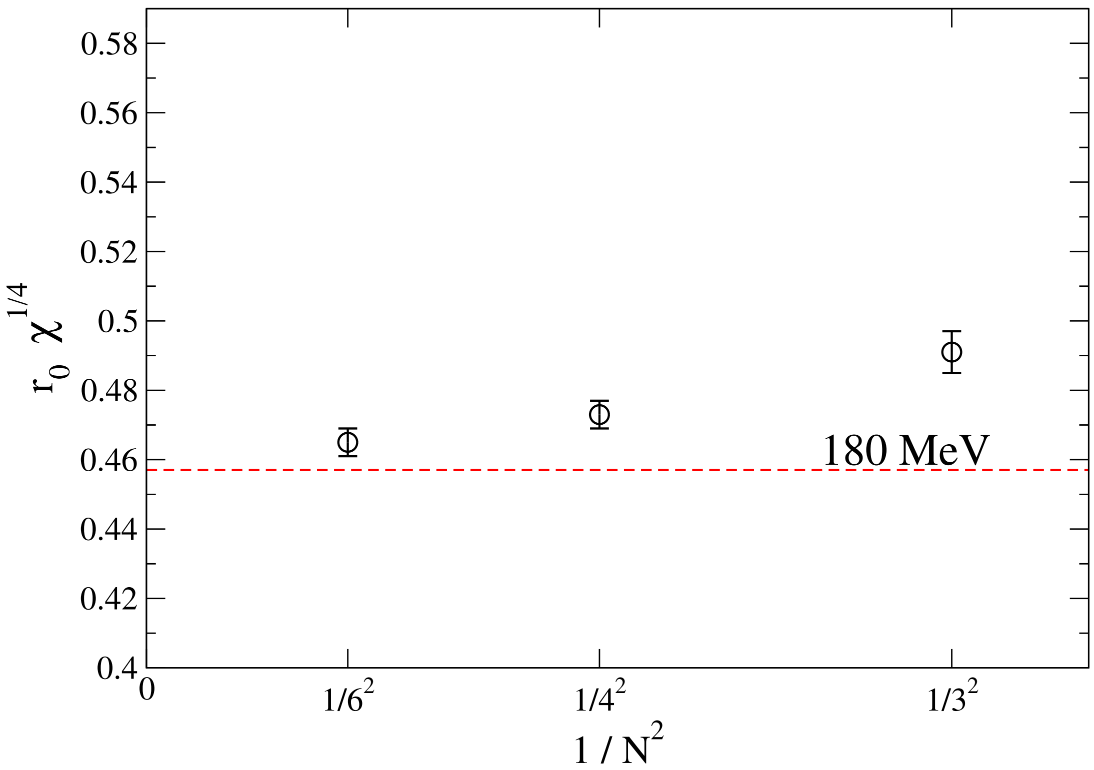
Fit to a constant: $\chi^2/d.o.f. = 4.93/5$

overall agreement and correct assessment of systematics



1. Subtraction of renormalizations: B. Alles, M. D'Elia and A. Di Giacomo, Nucl. Phys. B 494, 281-292 (1997), hep-lat/9605013, now rescaled by r_0 and continuum extrapolated
2. Latest cooling result: A. Athenodorou and M. Teper, arXiv:2007.06422
3. Wilson flow: M. Cè, M. García Vera, L. Giusti and S. Schaefer, PLB 762, 232-236 (2016), arXiv:1607.05939
4. Overlap fermions: L. Del Debbio, L. Giusti and C. Pica, PRL 94, 032003 (2005) hep-th/0407052
5. Spectral projectors (Wilson): M. Luscher and F. Palombi, JHEP 09, 110 (2010), arXiv:1008.0732
6. Spectral projectors (staggered): C. Bonanno, G. Clemente, M. D'Elia and F. Sanfilippo, JHEP 10, 187 (2019), [arXiv:1908.11832].

Large-N behaviour of χ



The topological susceptibility has a smooth and finite large-N limit

data from C. Bonati, M. D'Elia, P. Rossi and E. Vicari, Phys. Rev. D 94, no.8, 085017 (2016), arXiv:1607.06360

Large-N behaviour of $F(\theta)$?

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

(DIGA)

OR

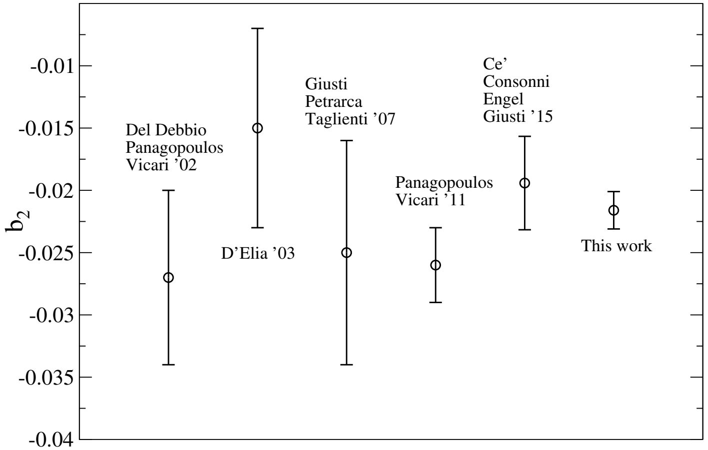
$$\Delta F(\theta) = F(\theta) - F(0) = \frac{\chi}{2}\theta^2 \left(1 + b_2\theta^2 + b_4\theta^4 + \dots\right)$$

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

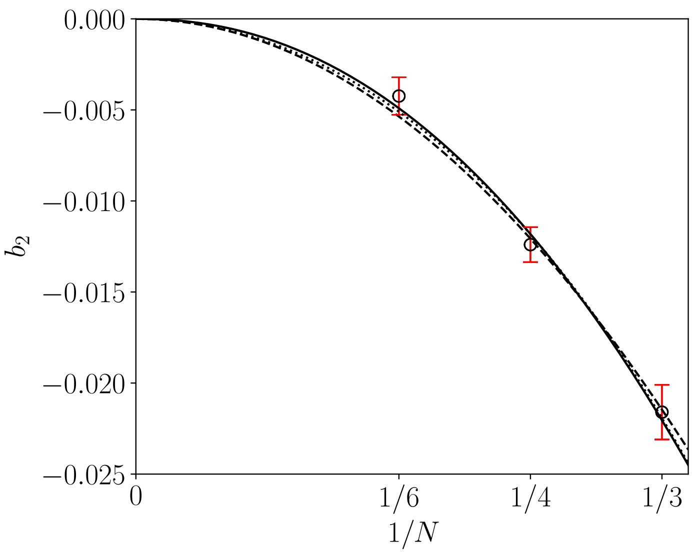
large-N Witten ansatz: scaling variable is θ/N

finite χ not compatible with DIGA, it is interesting anyway to test the scaling if further coefficients

Numerical results for b_2:



Most recent determination for $SU(3)$ (C. Bonati, M. D., A. Scapellato, 1512.01544) obtained by introducing an external imaginary θ source to improve signal/noise. Q measured by cooling.



Clear evidence for the predicted large-N scaling of b_2 (C. Bonanno, C. Bonati, M. D., 2012.14000)

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

recent improved determination obtained by a new algorithm which mitigates the topological freezing $\Longrightarrow$ $\bar{b}_2 = -0.193(10)$

What about finite temperature $SU(N)$?

- At a critical temperature $T_c \simeq 280$ MeV the theory undergoes a phase transition to a deconfined phase where center symmetry is spontaneously broken

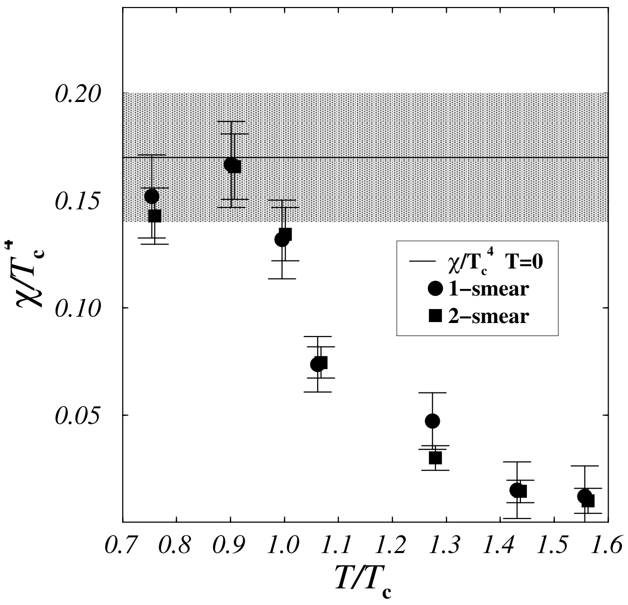
- At high enough temperature one expects a transition to a DIGA regime

$$F(\theta) \propto \cos\theta$$

  In principle that could happen at asymptotically high T where a perturbative expansion makes sense

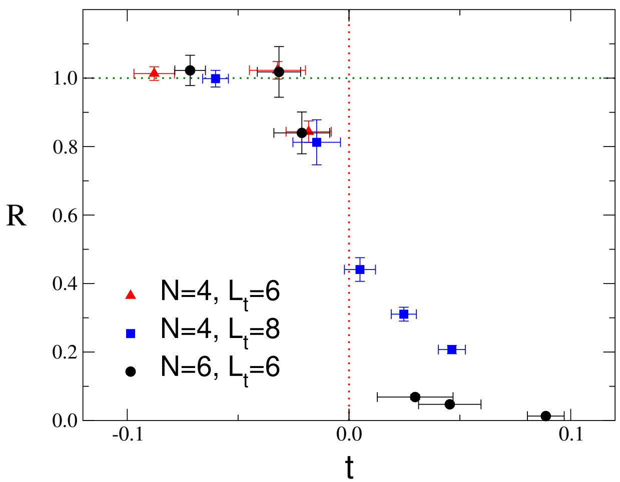
Any relation between the two transitions?

The topological susceptibility has a drop at T_c, sharper and sharper as N_c grows:



known for $SU(3)$ since long

B. Alles, M. D. and A. Di Giacomo, NPB 494, 281-292 (1997), hep-lat/9605013

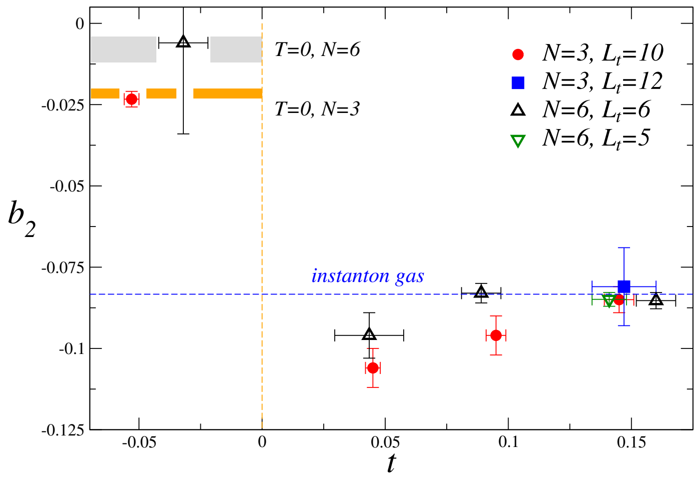


Large-N behavior around the transition

L. Del Debbio, H. Panagopoulos and E. Vicari, JHEP 09, 028 (2004), arXiv:hep-th/0407068

Drop of χ compatible with an effective DIGA regime, but not compelling. There are examples (e.g., $2dCP^{N-1}$ models), where DIGA does not work with a vanishing χ

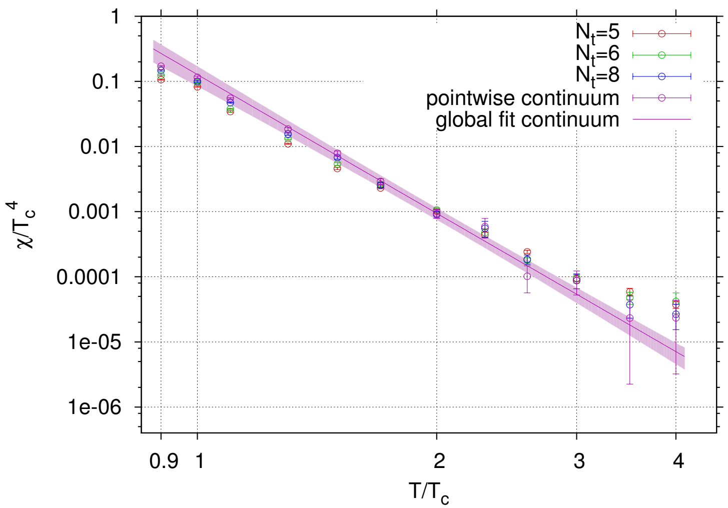
More compelling evidence from b_2 or from the power law drop of χ:



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 for $SU(N)$ pure Yang-Mills theories:

- 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 moving into the confined region, 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, lattice results, show a different situation: 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 $b_2 = -0.193(10)/N^2$, hence corrections must be significant.

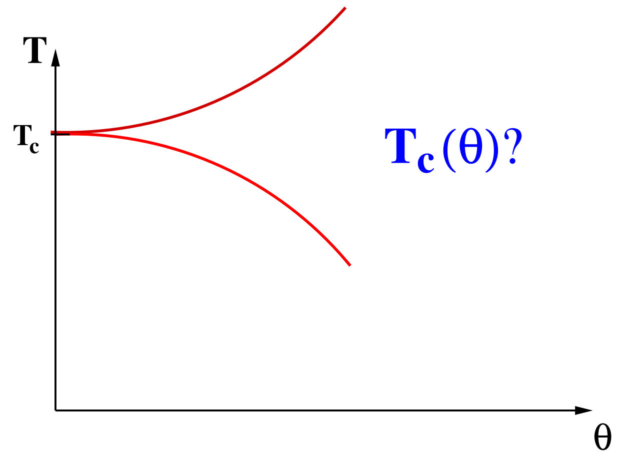
Let us now a consider a different, but related question

- can θ affect the location and nature of the transition? How does T_c changes if we switch a non-zero θ on?

We are looking for yet another extension of the QCD phase diagram, the θ-axis

We consider $SU(3)$ pure gauge theory

1^{st} order transition for $T_c(\theta = 0) \simeq 280$ MeV



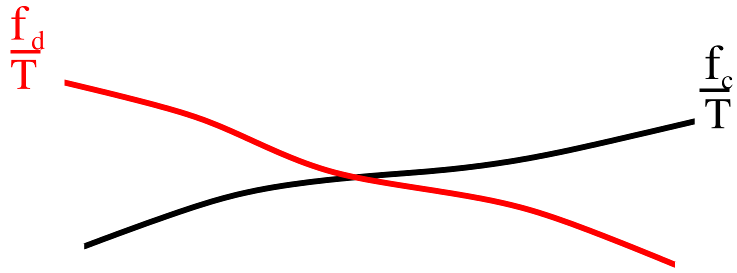
The theory is CP even at $\theta = 0 \implies T_c$ must be an even function of θ

Large N_c estimate

M. D. and F. Negro, PRL 109, 072001 (2012) 1205.0538

Main idea:

- Deconfinement transition is first order for $N_c \geq 3$, latent heat $\Delta\epsilon \propto N_c^2$
- We have two free energy density sheets (confined and deconfined) crossing at T_c



- Around T_c: $\quad \frac{f_c}{T} = A_c\, t + O(t^2) \qquad \frac{f_d}{T} = A_d\, t + O(t^2) \qquad t \equiv \frac{T-T_c}{T_c}$
- Latent heat: $\Delta\epsilon = -T^2\ \left[\partial(f_d/T)/\partial T - \partial(f_c/T)/\partial T\right]_{T_c} = T_c(A_c - A_d)$
- $\theta \neq 0$ shifts free energy $\quad f(T,\theta) = f(T,\theta=0) + \chi(T)\,\theta^2/2\ + O(\theta^4)$
  $\chi = \langle Q^2\rangle/V$ is the topological susceptibility

$\chi(T)$ differs in the two phases $\Longrightarrow$ the two sheets moves separately $\Longrightarrow$ T_c moves!

- **The equilibrium condition $f_c = f_d$ then reads**

$$A_c t + (\chi_c/T_c)\,\theta^2/2 \simeq A_d t + (\chi_d/T_c)\,\theta^2/2 \quad \Longrightarrow \quad t_c(\theta) = \frac{T_c(\theta)}{T_c(0)} - 1 = -\frac{\Delta\chi}{2\Delta\epsilon}\theta^2 + O(\theta^4)$$

- **We know that indeed $\chi(T)$ drops at the deconfinement transition!**
  In the large N_c limit the dependence simplifies (step function):
  - $\chi(T) = \chi(T=0) \equiv \chi$ **in the confined phase**
  - $\chi(T) = 0$ **in the deconfined phase**

- **leading N_c estimates** (B. Lucini, M. Teper, U. Wenger, 2004, 2005; H. Panagopoulos, E. Vicari, 2008)

$$\frac{\chi}{\sigma^2} \simeq 0.0221(14) \;\; ; \qquad \frac{\Delta\epsilon}{N_c^2 T_c^4} \simeq 0.344(72) \;\; ; \qquad \frac{T_c}{\sqrt{\sigma}} \simeq 0.5970(38)$$

$$\frac{T_c(\theta)}{T_c(0)} = 1 - R_\theta\,\theta^2 + O(\theta^4) \qquad R_\theta = \frac{\chi}{2\Delta\epsilon} \simeq \frac{0.253(56)}{N_c^2} + O(1/N_c^4)$$

A similar, decreasing behavior is also predicted by various effective models and semiclassical approximations (M. Unsal, 2012; E. Poppitz, T. Schäefer and M. Unsal, 2013; M. M. Anber, 2013; T. Sasaki, J. Takahashi, Y. Sakai, H. Kouno and M. Yahiro, 2011- 2012)

Lattice determination

QCD at finite θ is affected by a sign problem. We can borrow methods and strategies used to partially overcome the problem for QCD at finite baryon chemical potential μ_B

One possibility is analytic continuation: $\theta = i\,\theta_I \qquad Z(T,\theta_I) = \int [dA]\, e^{-S_{QCD} - \theta_I Q}$

$$\frac{T_c(\theta_I)}{T_c(0)} = 1 + R_\theta\, \theta_I^2 + O(\theta_I^4) \qquad \Longrightarrow \qquad \frac{T_c(\theta)}{T_c(0)} = 1 - R_\theta\, \theta^2 + O(\theta^4)$$

I will show you:

- a determination by analytic continuation (M. D. and F. Negro, PRL 109, 072001 (2012) 1205.0538)
- a comparison with reweighting in θ (M. D. and F. Negro, PRD 88, 034503 (2013) 1306.2919)

More recent work, with consistent results on the same topic, can be found in

N. Otake and N. Yamada, JHEP 06, 044 (2022) doi:10.1007/JHEP06(2022)044 [arXiv:2202.05605 [hep-lat]].

Lattice implementation

$$Z_L(T,\theta) = \int [dU]\, e^{-S_L[U]-\theta_L Q_L[U]}$$

$S_L = \beta \sum_{x,\mu>\nu}(1 - \mathrm{Re}\mathrm{Tr}\,\Pi_{\mu\nu}(x)/N) \quad \beta = 2N/g_0^2$ **(Wilson action)**

Which choice for $Q_L = \sum_x q_L(x)$?

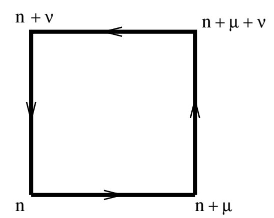
- **A gluonic definition tipically leads to renormalizations**

  $q_L(x) \overset{a\to 0}{\sim} a^4 Z(\beta) q(x) + O(a^6) \quad \Longrightarrow \quad \theta_I = Z(\beta)\,\theta_L + O(a^2)$

- **A fermionic, renormalization free definition (e.g. based on overlap operators) would lead to unreasonable computational requirements**

Optimal Strategy: **simplest gluonic definition (no smearing) so that heat-bath + over-relaxation works, then compute the multiplicative renormalization** $Z(\beta)$

$q_L(x) = \frac{-1}{2^9\pi^2} \sum_{\mu\nu\rho\sigma=\pm 1}^{\pm 4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \mathbf{Tr}\,(\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)) \qquad \Pi_{\mu\nu} \rightarrow$



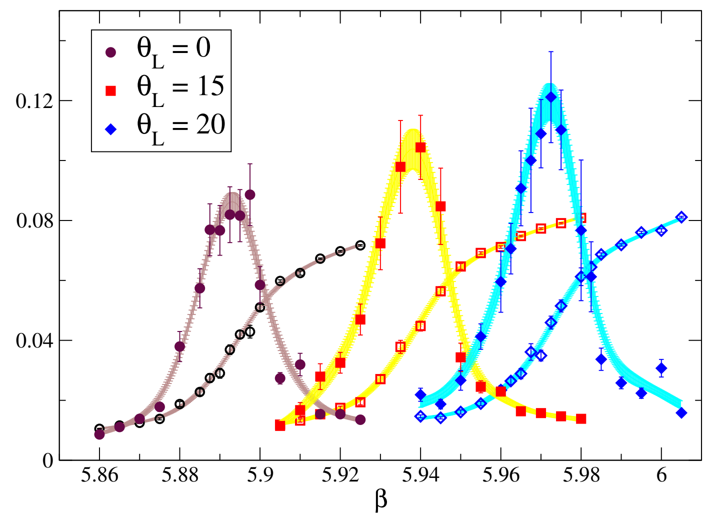
Locating the phase transition

$Z(N)$ center symmetry, which is spontaneously broken at the deconfinement transition of pure $SU(N)$ gauge theories, is still exact in presence of a θ term.

$\Longrightarrow$ The Polyakov loop is still a good order parameter to locate deconfinement

$$\langle L \rangle \equiv \frac{1}{V_s} \sum_{\vec{x}} \frac{1}{N} \langle \mathrm{Tr} \prod_{t=1}^{N_t} U_0(\vec{x}, t) \rangle \qquad \chi_L \equiv V_s \left(\langle L^2 \rangle - \langle L \rangle^2 \right) ,$$

Polyakov loop and its susceptibility as a function of β for $N_t = 6$ and a few θ_L



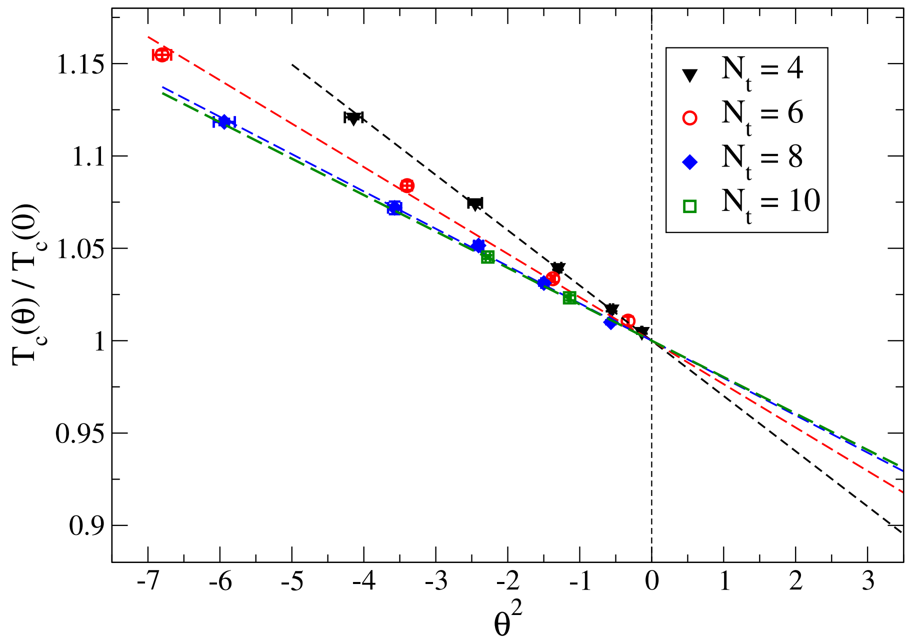
$\beta_c(\theta_L)$ located at the peak of χ_L

$$\beta_c(\theta_L) \quad \longrightarrow \quad T_c(\theta_L) = \frac{1}{N_t \, a(\beta_c(\theta_L))}$$

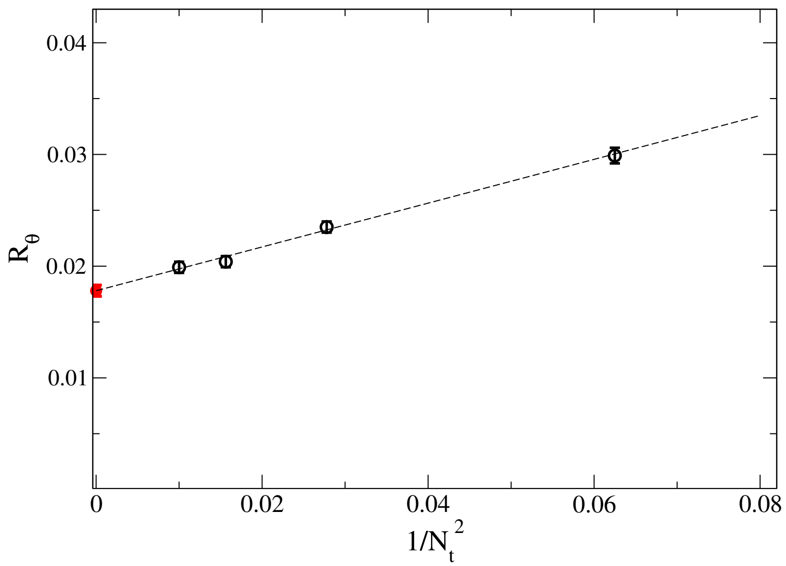
Best fit to

$$T_c(\theta)/T_c(0) = 1 - R_\theta\,\theta^2$$

for data at different values of N_t



Continuum extrapolation ($N_t \to \infty$**) assuming** $O(a^2)$ **corrections (**$\chi^2/\mathrm{d.o.f.} \simeq 0.97$**)**

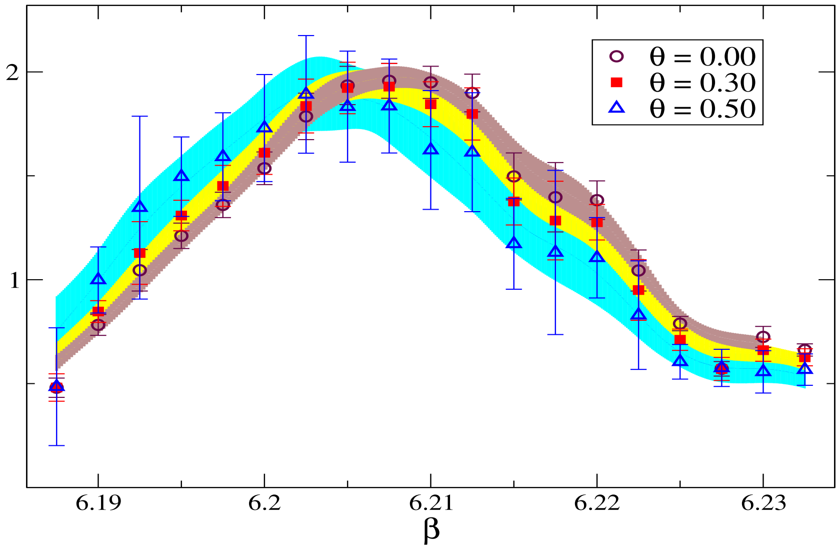


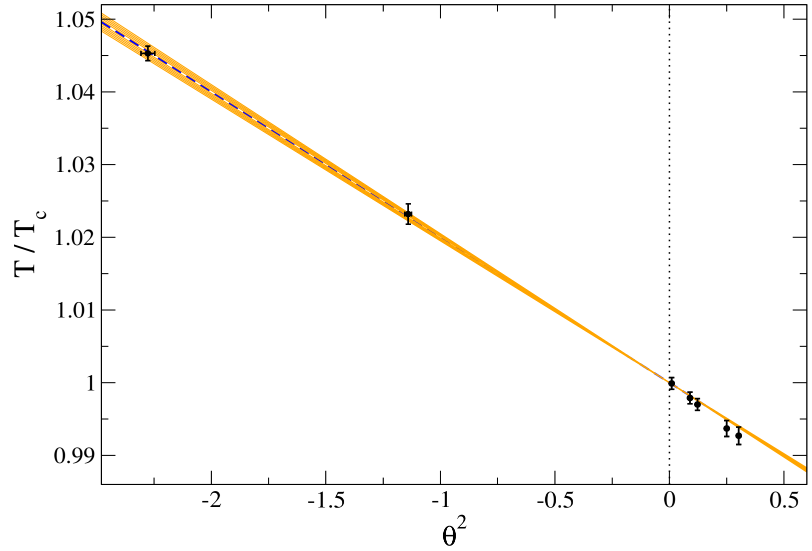
$$R_\theta^{cont} = 0.0178(5)$$

large N_c **estimate is a bit larger:** $R_\theta \simeq 0.0281(62)$ **but indeed** $\chi(T)$ **does not drop to zero at** T_c **for** $N_c = 3$**.**

Analytic continuation vs. Reweighting

Location of T_c





LEFT: Polyakov loop susceptibility for different real θ

RIGHT: $T_c(\theta)$: extrapolation from imaginary θ compared to reweighting.

$$\langle O \rangle_\theta = \frac{\int [dU]\, e^{-S_L[U]+i\theta Q}\, O}{\int [dU]\, e^{-S_L[U]+i\theta Q}} = \frac{\langle e^{i\theta Q} O \rangle_{\theta=0}}{\langle \cos(\theta Q) \rangle_{\theta=0}} \, .$$

Results from reweighting are compatible with those from analytic continuation

Sketching the $T-\theta$ phase diagram

M. D. and F. Negro, PRD 88, 034503 (2013)

- **low-T dependence is on θ/N (Witten). Periodicity in θ restored by first order phase transitions at $\theta=(2k+1)\pi$ (multi-branched vacuum energy)**

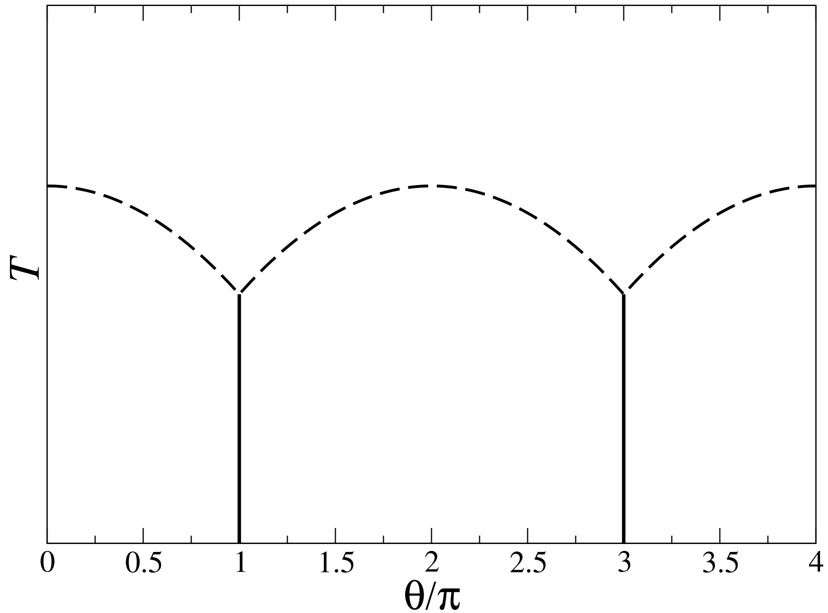
- **high-T dependence of the free energy is on θ, from semiclassical instanton computations. Lattice simulations show that this actually happens right after T_c**

  Free energy dependence is smoothly periodic in θ in the high T regime.

- **$T_c(\theta)$ itself depends on θ/N, and could be dominated, at large N, by the quadratic term down to $\theta=\pi$. Most likely, it is a multibranched function as well**

$$\frac{T_c(\theta)}{T_c(0)} \simeq 1 - R_\theta \min_k (\theta+2\pi k)^2 \qquad R_\theta \sim \frac{1}{N_c^2}$$

This is the resulting conjectured phase diagram



There is, actually, a further unjustified assumption: **the critical line $T_c(\theta)$ touches the low-T transition present at $\theta = \pi$ exactly at its endpoint.**

Conclusions

Numerical results for pure gauge $SU(N)$ gauge theories provide a clear picture, consistent with available expectations and suggesting a strict relation between confining/deconfining properties and θ-dependence.

Moreover, θ itself enhances the onset of deconfinement

A few interesting topics have not been covered in this talk:

- Numerical study of θ-dependence in 2D CP^{N-1} models, where precise analytical predictions exist

  C. Bonanno *et al* arXiv:1807.11357, arXiv:1911.03384, arXiv:2009.14056

  C. Bonanno, MD, F. Margari, explicit numerical evidence of topological susceptibility divergence for $N = 2$, on arXiv tomorrow

- Closer look at the relation between θ-dependence and center symmetry realization in trace deformed Yang-Mills theories M. Cardinali *et al* arXiv:1807.06558, arXiv:1912.02662, arXiv:2010.03618, arXiv:2012.13246