θ dependence in QCD

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Electroweak, Strong and New Interactions: a symposium to celebrate Guido's 70th birthday

Rome, 26 September 2022

OUTLINE

- **θ-dependence in QCD: motivation and predictions**

- **θ-dependence from lattice QCD: main challenges**

- **Well established results for $SU(N)$ pure gauge theories**

- **Open challenges for full QCD: where my path met Guido's**

Many non-perturbative properties of strong interactions are related to the topological classification of the QCD path integral

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

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

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

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

Homotopy group: $\pi_3(SU(N)) = \mathbb{Z}$

$G\tilde{G}$ **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.

Since Q is integer valued, θ behaves like an angular variable. Non-trivial θ-dependence emerges because of the existence of configurations with finite action and $Q \neq 0$ (e.g., classical solutions: instantons and anti-instantons)

From a lattice QCD perspective, numerical computations at $\theta \neq 0$ are made difficult by the appearance of a complex factor in the path-integral: sign problem

we can only access a small region around $\theta = 0$ by a Taylor expansion approach

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

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

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

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

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

$\psi_f \to e^{i\alpha\gamma_5}\psi_f, \;\; \bar{\psi}_f \to \bar{\psi}_f e^{i\alpha\gamma_5}$ $\Longrightarrow$ $\theta \to \theta - 2\alpha$ **and the mass matrix becomes complex**

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?

- **It enters phenomenology anyway, like in Witten-Veneziano mechanism for the η' mass:**

$$\chi^{YM}_{N=\infty} = \frac{f_\pi^2}{2N_f}\left(m^2_{\eta'} + m^2_{\eta} - 2m^2_K\right) \quad \Longrightarrow \quad \chi^{YM}_{N=\infty} \simeq (180\ \mathrm{MeV})^4$$

- **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, the QCD axion, which is also a dark matter candidate and whose properties are largely fixed by θ-dependence

The QCD axion

Main idea: add a new scalar field acquiring a VEV which breaks a $U(1)$ symmetry (Peccei-Quinn). Various high energy models exist, low energy effective lagrangian:

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

- $a \sim$ Goldstone boson, with only derivative terms apart from a coupling to $G\tilde{G}$.

- shifting $\langle a \rangle$ shifts θ by $\langle a \rangle / f_a$. However θ-dependence of QCD breaks the shift symmetry 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

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

θ-dependence at finite T fixes axion parameters during the Universe evolution

Predictions about θ-dependence - I

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

Integration around classical solutions yields the one-instanton contribution $\propto e^{-8\pi^2/g^2(\rho)}$

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

- by asymptotic freedom, works well for small instantons, which are then exponentially suppressed and dilute, making the single instanton computation correct **(DIGA)**

- the presence of large instantons ($1/\rho \lesssim \Lambda_{QCD}$) in general breaks DIGA.

- however, DIGA may work well only in the presence of an effective IR cutoff, like a finite temperature $T > \Lambda_{QCD}$ which suppresses large instantons.

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**

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

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

should be valid as soon as instantons and anti-instantons are dilute enough

- **Perturbative prediction for $\chi(T)$:**

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

should be valid for large enough temperatures

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 the 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 $N_c \to \infty$

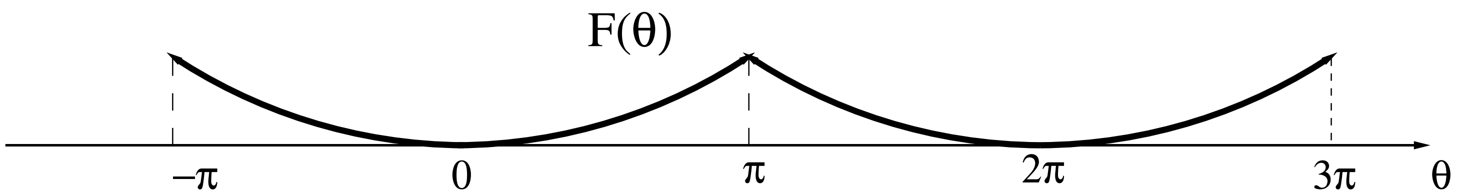
Large-N_c scaling: consequences

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

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 $\theta = (2k+1)\pi$



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)

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

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

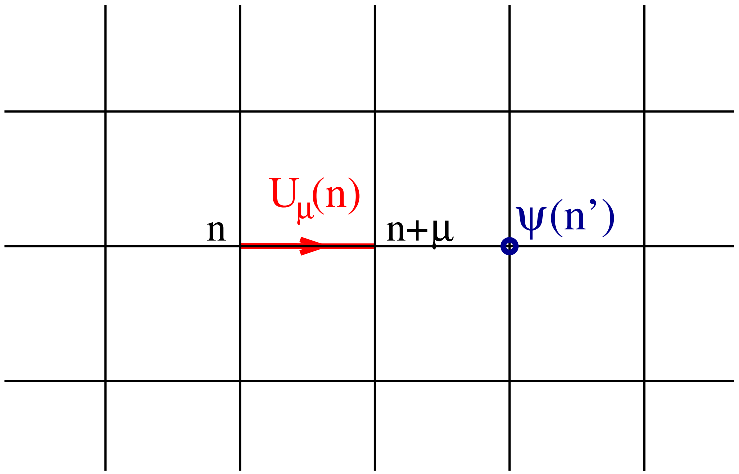
Explicitly

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

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

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



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, the fermion matrix $M[U]$ is some discretized version of $D_\mu \gamma_\mu + m_q$

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

- Is topology well defined? The concept of homotopy classes is recovered only for smooth, semiclassical configurations. Standard discretizations of $G\tilde{G}$ need renormalizations

- Are the chiral properties of discretized fermions good enough to correctly identify zero modes? **(both for measurement and for sampling!)**

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

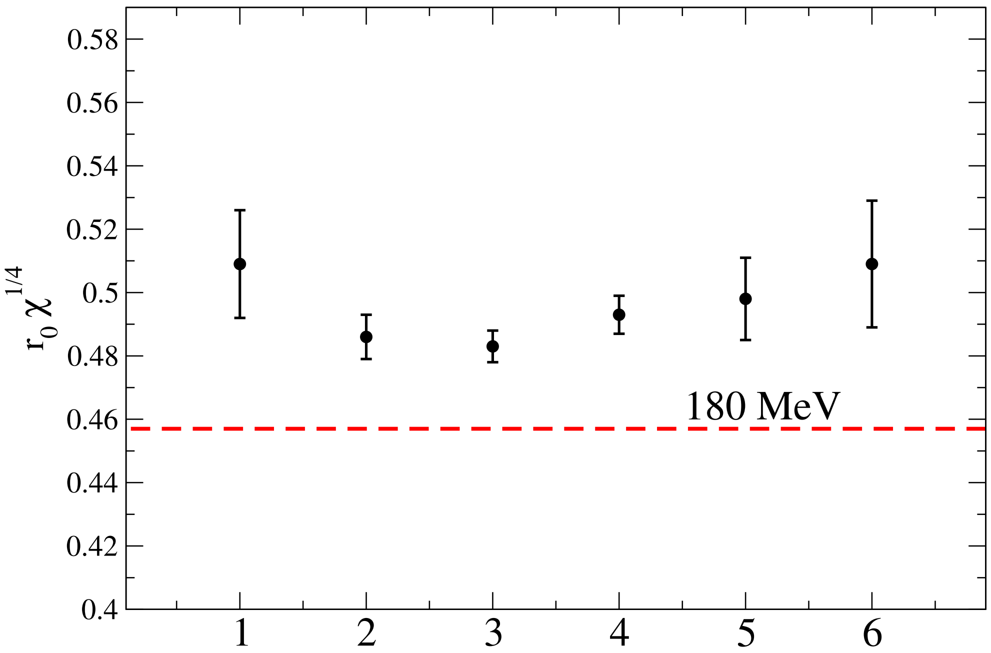
- **Algorithmic issues: critical slowing down and sampling of rare events**
  - in the continuum limit, homotopy classes are no more connected by finite action configurations. Algorithms may lose ergodicity
  - in a finite volume, it may happen that $\langle Q^2 \rangle = \chi V \ll 1$. One may need 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)

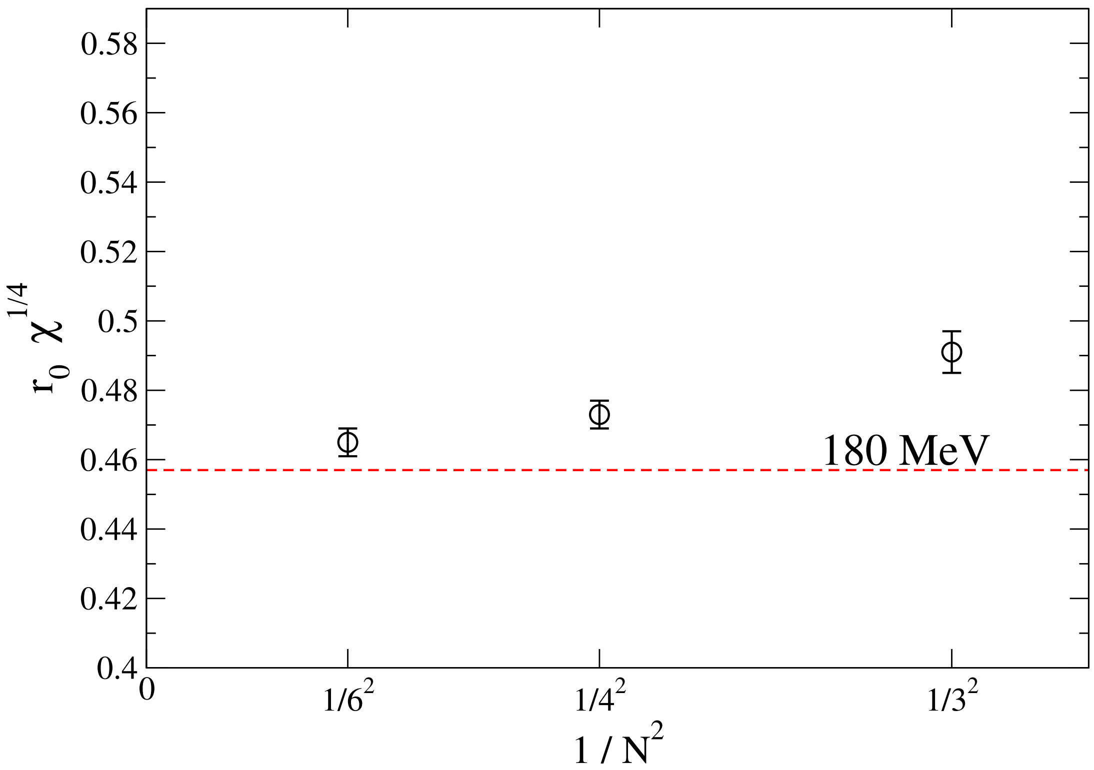
Fit to a constant: $\chi^2/d.o.f. = 4.93/5$

overall agreement and correct assessment of systematics



1. Subtraction of renormalizations: B. Alles, MD 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, MD and F. Sanfilippo, JHEP 10, 187 (2019), [arXiv:1908.11832].

Large-N behaviour of χ

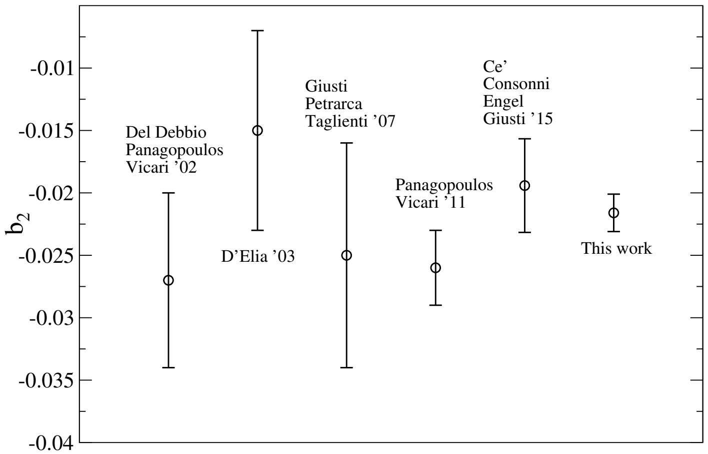


The topological susceptibility has a smooth and finite large-N limit

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

A finite χ at large N falsifies DIGA at $T = 0$

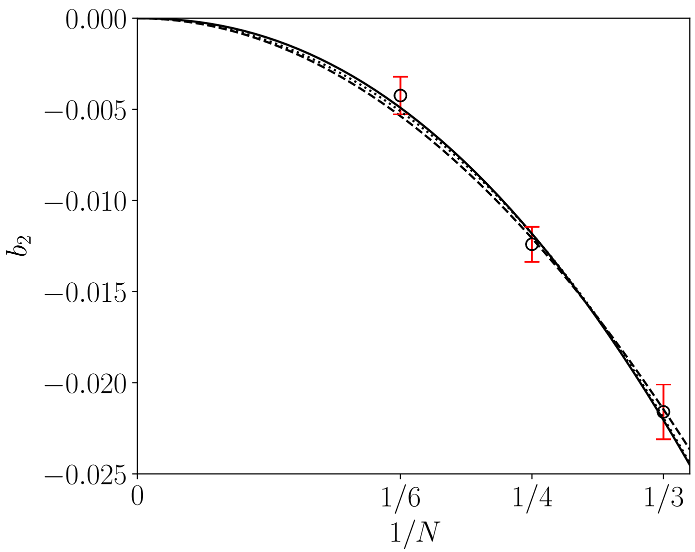
Further evidence of large-N Witten scaling from higher order cumulants



Most recent determinations for $SU(3)$ of the cumulant

$$b_2 \equiv -\frac{\langle Q^4 \rangle_c}{12 \langle Q^2 \rangle}$$

(last point from Bonati, MD, Scapellato, 1512.01544)



Clear evidence for the predicted large-N scaling of b_2 (Bonati, MD, Rossi, Vicari, 1607.06360)

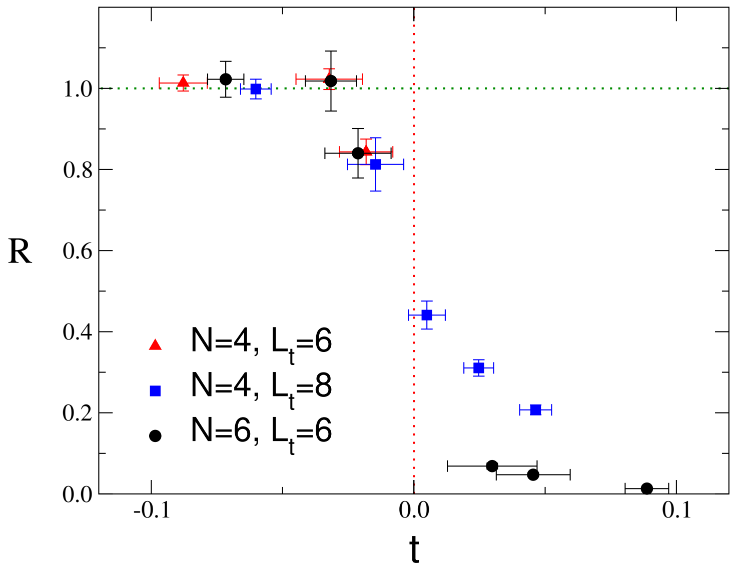
$$b_2 \simeq \frac{\bar{b}_2}{N^2}$$

recent determination by a new algorithm which mitigates topological freezing $\Longrightarrow$ $\bar{b}_2 = -0.193(10)$ (Bonanno, Bonati, MD, 2012.14000)

DIGA recovered at high temperature? At which scale?

any relation with the deconfining temperature $T_c \simeq 280$ MeV?

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



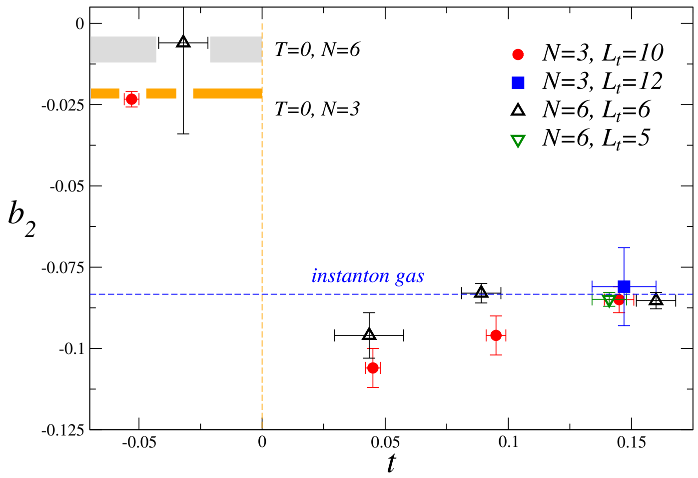
Large-N behavior around the transition

L. Del Debbio, H. Panagopoulos and E. Vicari, hep-th/0407068

$$t \equiv \frac{T - T_c}{T_c} \; ; \qquad R \equiv \frac{\chi(T)}{\chi(T=0)}$$

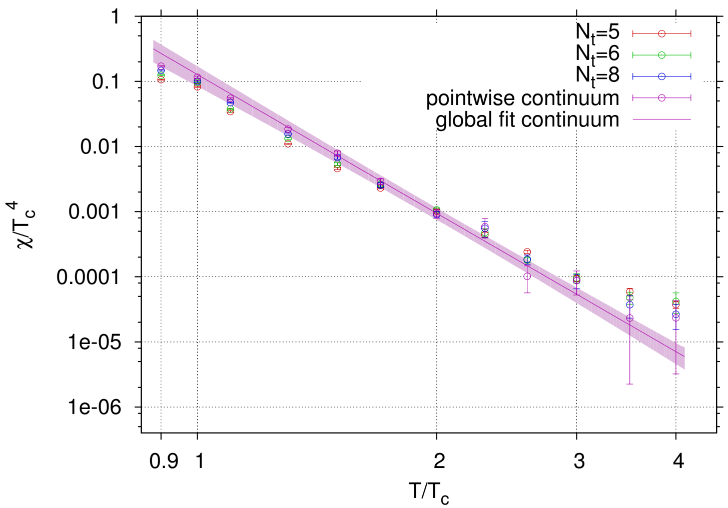
The sharp drop of χ suggests the onset of a DIGA regime soon after T_c

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 $T \gtrsim 1.1\, T_c$.



from S. Borsanyi et al. 1508.06917

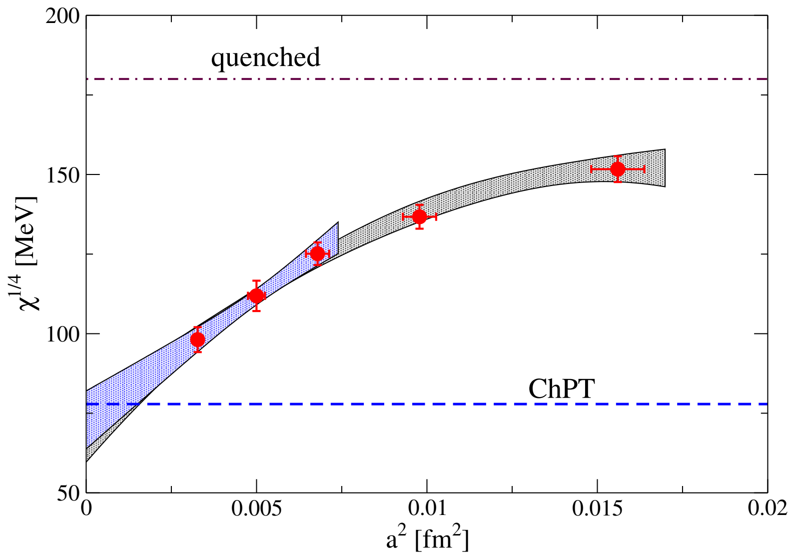
The perturbative power law behavior predicted for χ at high T has been verified

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

Let us switch now to full QCD results

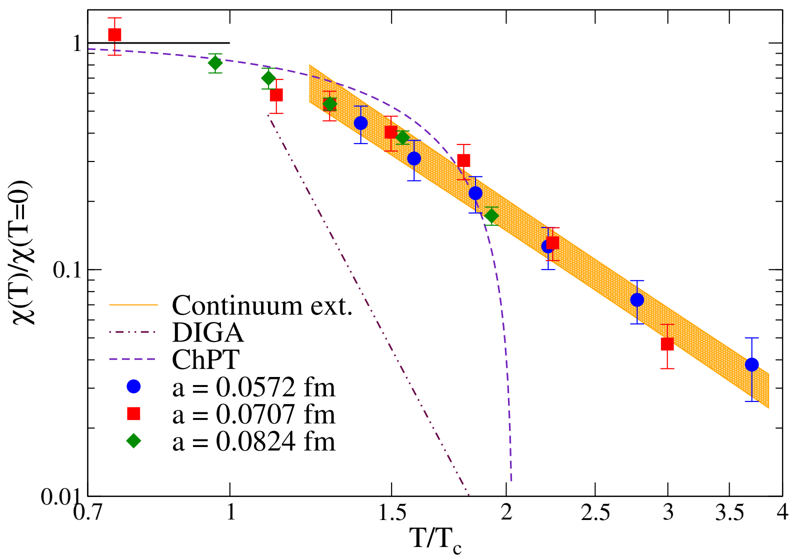
C. Bonati, MD, M. Mariti, G. Martinelli, M. Mesiti, F. Negro, F. Sanfilippo and G. Villadoro, 1512.06746

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



slow approach to continuum because of slow approach to chiral properties of fermions

zero modes are not exact, $\det M$ does not properly suppress $Q \neq 0$ configurations



finite T results showed a drop of $\chi(T)$ much smoother than perturbative estimate

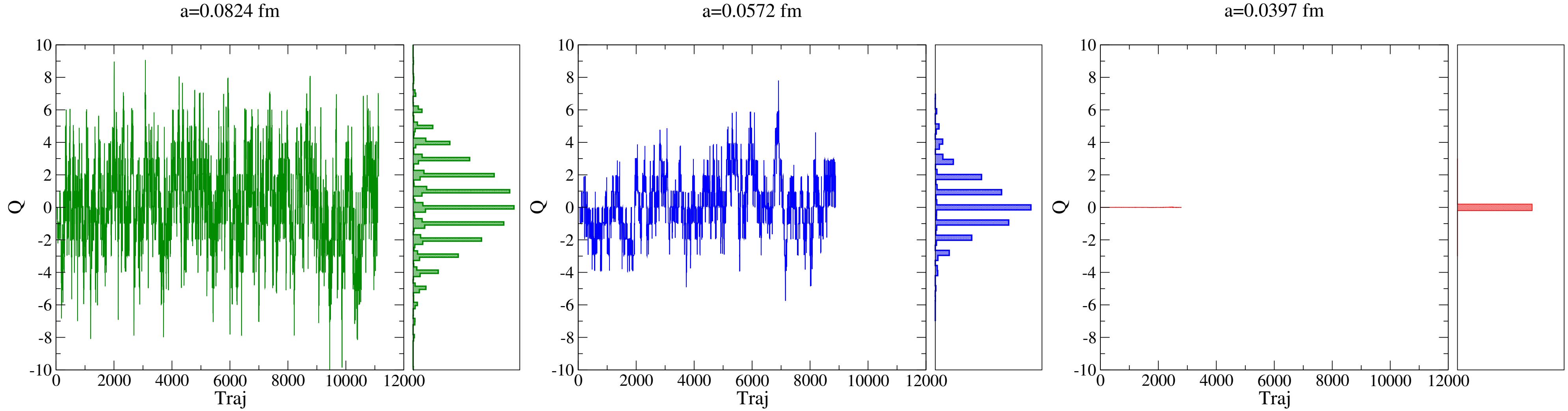
$\chi(T) \propto 1/T^b$ **with** $b = 2.90(65)$ **(DIGA prediction:** $b = 7.66 \div 8$**)**

resulting in a larger predicted axion mass

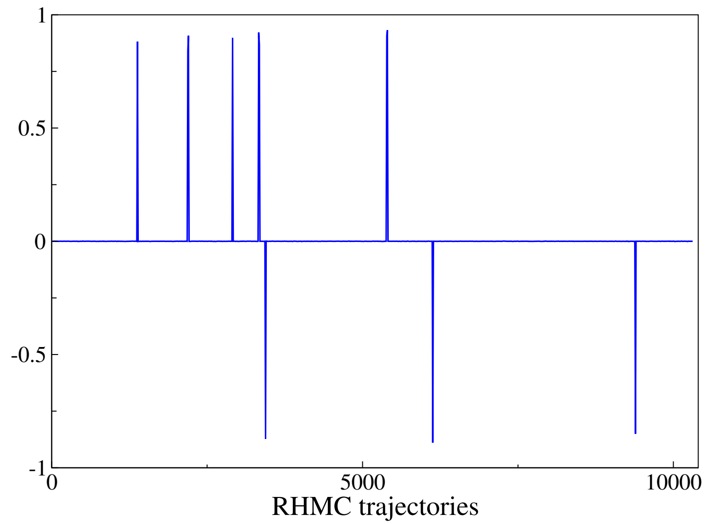
However UV artifacts were still quite large ...

Algorithmic problems: topological freezing at small a and difficult sampling of rare events at high T

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



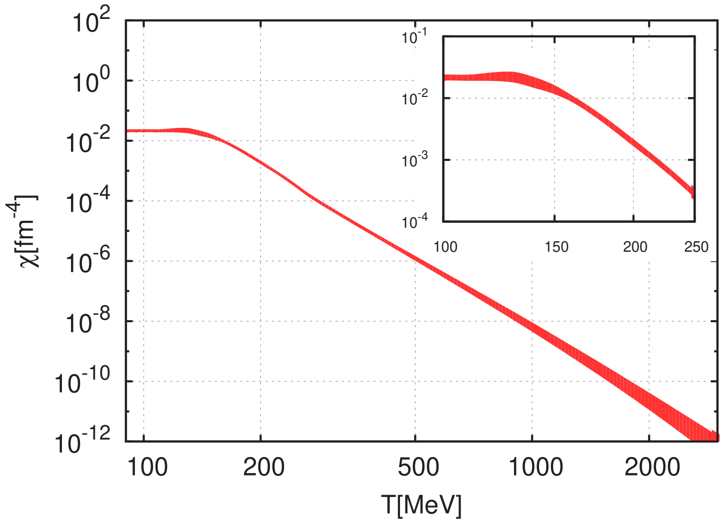
Evolution of Q in MC time for an high T simulation of $N_f = 2+1$ QCD, $\langle Q^2 \rangle \sim 10^{-3}$.



Finite T results for $N_f = 2 + 1$ QCD: why is it difficult?

three monsters to defeat at the same time

1. discretization effects with physical quark masses: requires small lattice spacing
2. topological freezing at small lattice spacing
3. correct sampling of extremely rare topological modes at very high T



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

DIGA power law OK; $m_a(\text{today}) \sim$ 100 μeV

with some approximations:

- simulations at fixed Q, in practice only $P(Q=1)/P(Q=0)$ is computed
- reweighting of configurations a posteriori by $m_f/|m_f + i\lambda|$ to force zero modes by hand

Any systematics related to that?

Defeating the rare event problem by a multicanonical approach

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

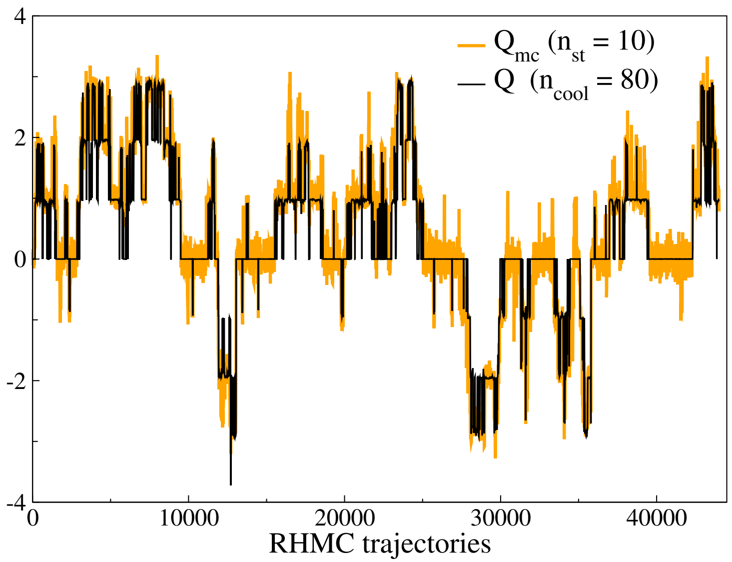
The idea is to modify the probability distribution, by adding a Q dependent potential to the action and then reweight

$$\langle Q^2 \rangle = \frac{\int \mathcal{D}U e^{-S_{QCD}}\, Q^2}{\int \mathcal{D}U e^{-S_{QCD}}} = \frac{\int \mathcal{D}U e^{-S_{QCD}-V(Q)}\, Q^2 e^{V(Q)}}{\int \mathcal{D}U e^{-S_{QCD}}} = \frac{\langle Q^2 e^{V(Q)} \rangle_V}{\langle e^{V(Q)} \rangle_V}$$

If $V(Q)$ is chosen so as to enhance high Q configurations, the rare events will be sampled more frequently and then correctly reweighted. The improvement in the statistical error can be impressive.

A similar strategy is adopted in metadynamics, where $V(Q)$ is made dynamical

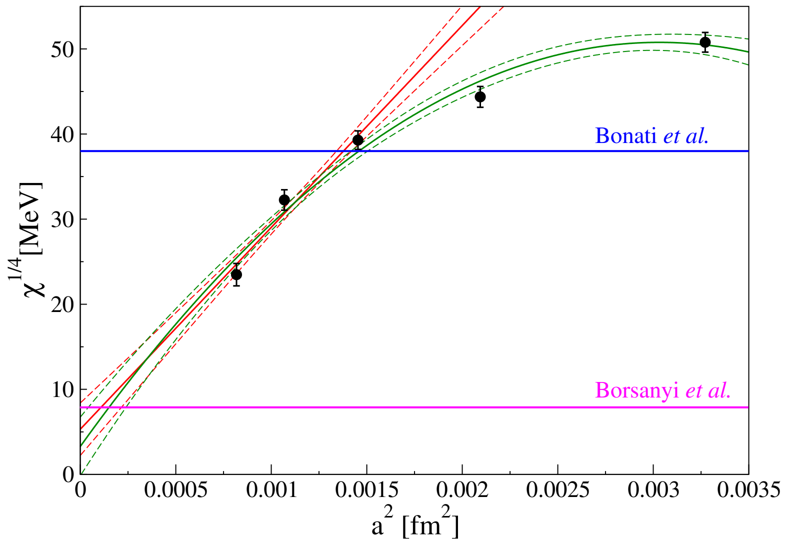
(A. Laio, G. Martinelli and F. Sanfilippo, arXiv:1508.07270)



As the lattice spacing decreases, χ drops down and the gain increases

$48^3 \times 16$ **lattice,** $a = 0.0286$, $T = 430$ **MeV**

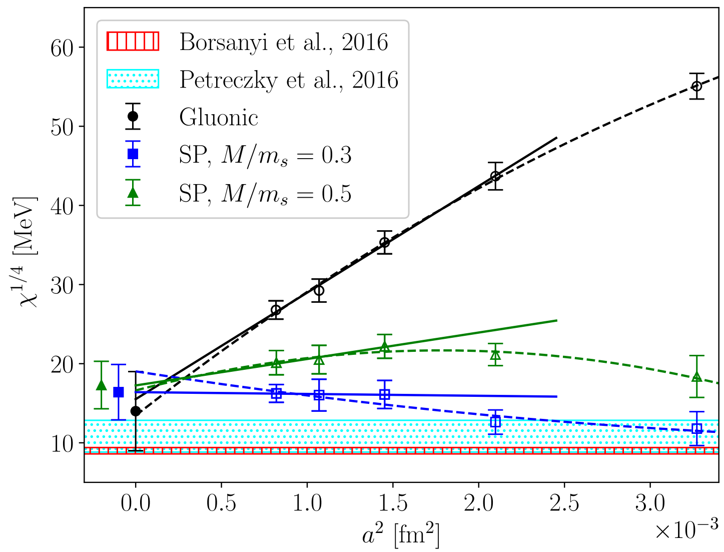
In this case $\langle Q^2 \rangle = 2.1(7) \times 10^{-4}$ **and the estimated gain is** $O(10^3)$**.**



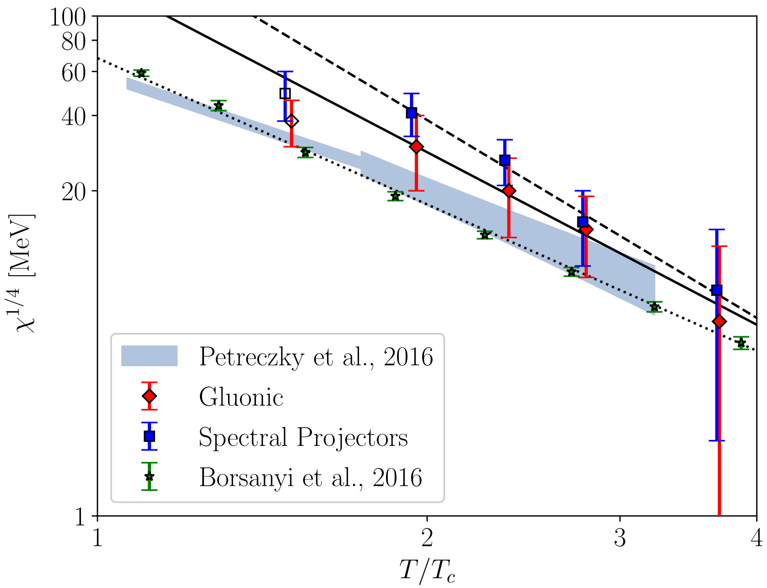
However, UV corrections are still significant, leading to a continuum extrapolation with large uncertainties

Improving on UV corrections by spectral projectors

A. Athenodorou, C. Bonanno, C. Bonati, G. Clemente, F. D'Angelo, MD, L. Maio, G. Martinelli, F. Sanfilippo and A. Todaro, arXiv:2208.08921



A fermionic definition of Q based on the same Dirac operator used for sampling configurations (staggered spectral projectors) leads to reduced lattice artifacts and improved estimates.



The behavior of $\chi(T)$ is now in good agreement with DIGA exponents for $T \gtrsim 300$ MeV

$\chi(T) \propto 1/T^b$ with $b = 10(3)$ (DIGA prediction: $b = 7.66 \div 8$)

some tension with previous lattice results, to be clarified ...

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.

- **Large-N Witten scaling below T_c**
- **rapid onset of DIGA above T_c.**

The investigation of QCD at the physical point still represents a challenge and will require more computational and algorithmic efforts in the future

Guido, we have still a long way to go on these topics!

Happy Birthday Guido!