Phase structure of Yang-Mills theories in the presence of a θ term

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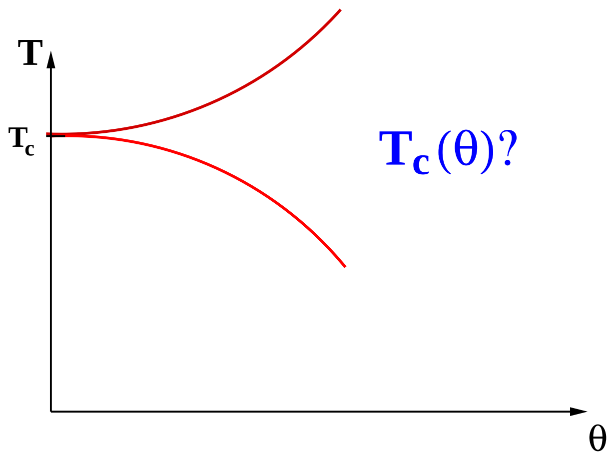
1 – Introduction

- **We know that θ-dependence of the QCD free energy changes drastically at T_c.**
- **Here we start with a different, 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, and for new troubles with another sign problem

We consider $SU(3)$ pure gauge theory

1^{st} **order transition for $T_c(\theta = 0) \simeq 270$ MeV**



$$Z(T,\theta) = \int [dA]\, e^{-S_{QCD}[A]+i\theta Q[A]} = e^{-V_s f(\theta)/T} \qquad Q = \int d^4x \frac{g_0^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x)$$

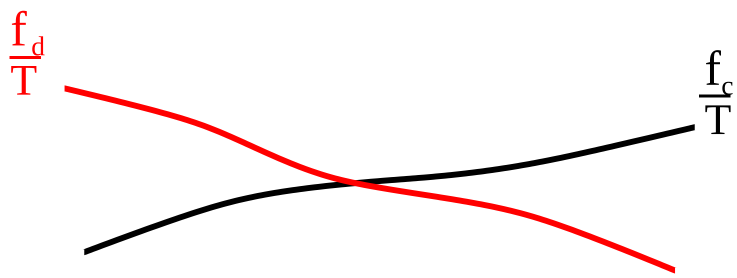
The theory is CP even at $\theta = 0$ $\Longrightarrow$ T_c must be an even function of θ

We have some prediction: 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: $\frac{f_c}{T} = A_c\, t + O(t^2)$ $\frac{f_d}{T} = A_d\, t + O(t^2)$ $t \equiv \frac{T-T_c}{T_c}$
- 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 $f(T,\theta) = f(T,\theta=0) + \chi(T)\,\theta^2/2\ + O(\theta^4)$
  $\chi = \langle Q^2\rangle/V$ 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 semi-classical 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)**

2 – Lattice determination

We can borrow methods and strategies used to partially overcome the sign problem for QCD at finite baryon chemical potential μ_B

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

Azcoiti *et al*, hep-lat/0203017; Allés - Papa 0711.1496; S. Aoki *et al*, 0808.1428; Panagopoulos - Vicari, 1109.6815

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

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)**

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 $Q_L = \sum_x q_L(x)$?

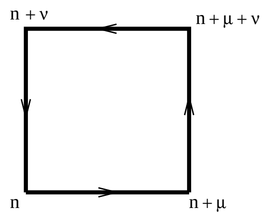
- **A gluonic definition tipically leads to renormalizations**

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

- **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 $Z(\beta)$**

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



Simulation parameters

- **four different lattice spacings:**
  $a \sim 1/(N_t T_c) = 1/(4T_c), 1/(6T_c), 1/(8T_c), 1/(10T_c)$ $(0.18 \rightarrow 0.07\ \mathrm{fm})$ **in order to perform the continuum limit extrapolation**

- **four different lattices with equal physical spatial volume:**
  $16^3 \times 4$, $24^3 \times 6$, $32^3 \times 8$, $40^3 \times 10$

- **we determine $T_c(\theta_I)/T_c(0)$:**
  most finite size effects are expected to cancel out in the ratio

- **Typical statistics:**
  $10^5 - 10^6$ **MC sweeps for each θ_L , β**
  Autocorrelation times up to 10^3 at the transition.

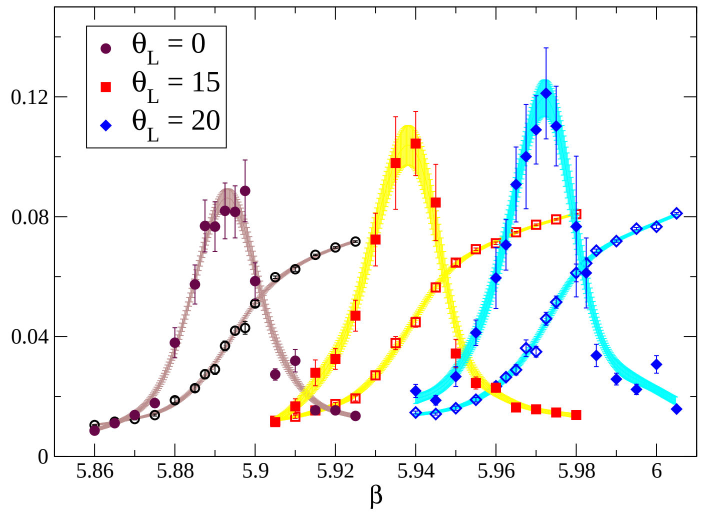
Locating the phase transition

$Z(N)$ **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

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

non perturbative $a(\beta)$ **from G. Boyd *et al.*, Nucl. Phys. B 469, 419 (1996).**

Renormalization: $T_c(\theta_I = Z\theta_L)$ $\quad Z = Z(\beta_c(\theta_L))$

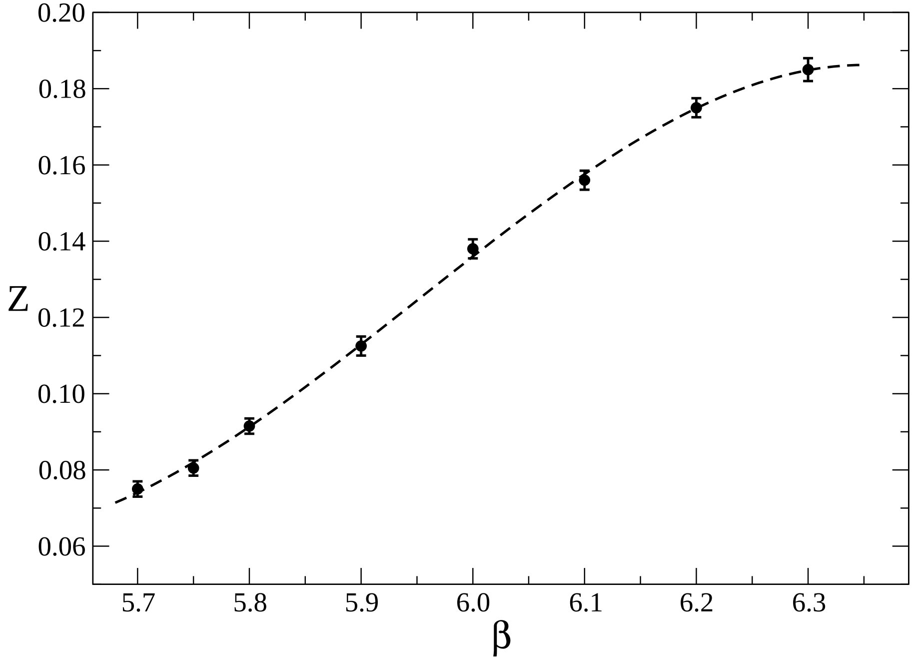
Non-perturbative methods to determine Z exploit the fact that UV fluctuations responsible for renormalization are independent of the topological background:

- $Z = \langle Q_L \rangle_Q / Q$ **in a fixed backgroud Q (heating techniques)**
- $Z = \langle Q_L Q \rangle / \langle Q^2 \rangle$ **over all configurations, where Q is determined by cooling or fermionic methods (Panagopoulos-Vicari 2011)**

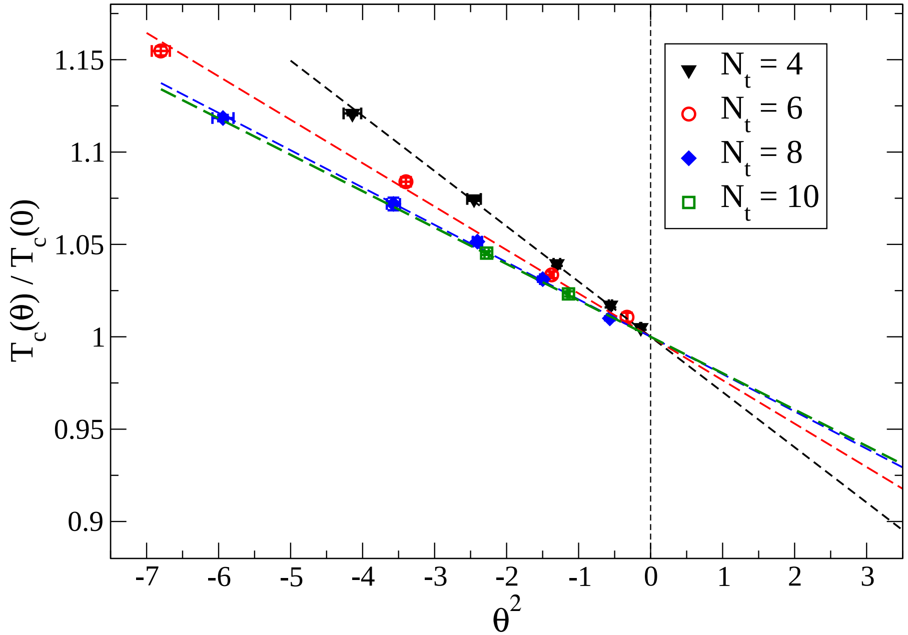
We adopt the second strategy

$\frac{\langle Q_L Q \rangle}{\langle Q^2 \rangle}$ **determined on $O(10^5)$ configurations for each β (by cooling)**

$Z(\beta)$ **for intermediate $\beta' s$ by cubic interpolation**



We can now try best fits to interpolate data at $\theta^2 < 0$, then extrapolate to $\theta^2 > 0$

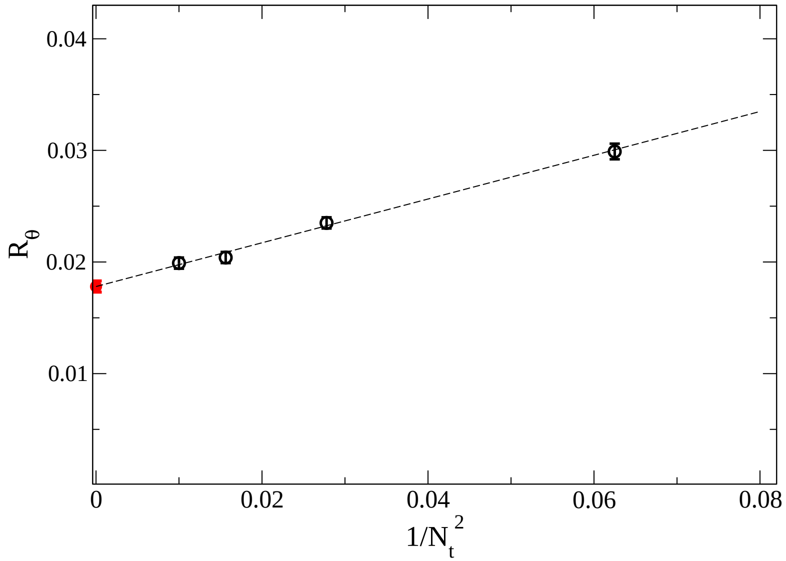


The quadratic fit

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

works well ($\chi^2/\text{d.o.f.} \lesssim 1$)

and is stable in all the explored range.



We extrapolate to $N_t = \infty$ assuming $O(a^2)$ corrections ($\chi^2/\text{d.o.f.} \simeq 0.97$)

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

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 $N_c = 3$.

3 – Cross-checking with reweighting

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

Usually one needs to compare different approximate solutions to a sign problem in order to get confident of systematic effects. One possibility is reweighting in θ

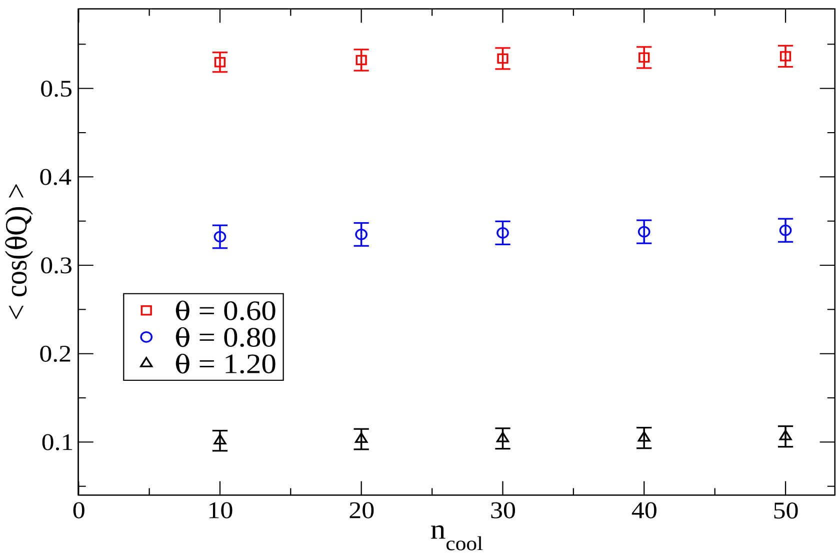
$$\langle O \rangle_\theta = \frac{\int [dU]\, e^{-S_L[U]+i\theta Q}\, O}{\int [dU]\, e^{-S_L[U]+i\theta Q}} = \frac{\langle e^{i\theta Q} O \rangle_{\theta=0}}{\langle \cos(\theta Q) \rangle_{\theta=0}}\,.$$

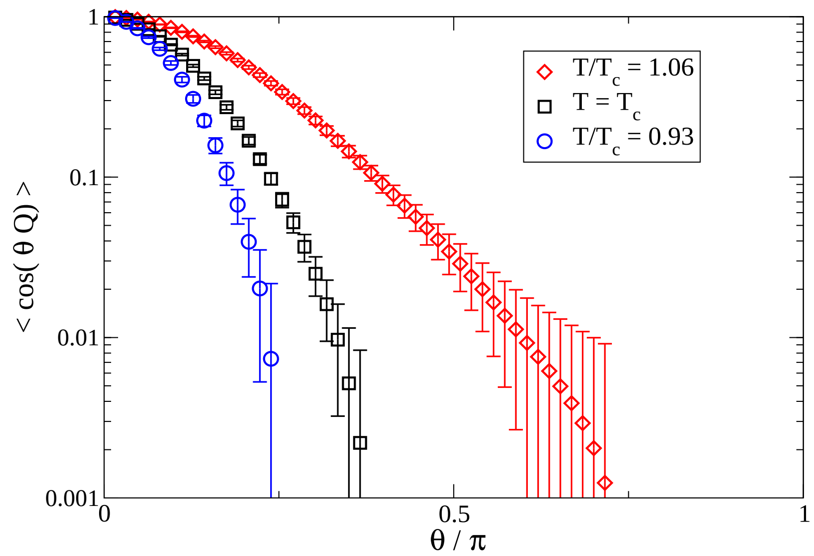
here Q is the topological background, measured configuration by configuration, hence θ does not need renormalization in this approach

The comparison is performed on the finest lattice ($40^3 \times 10$): $a \sim 0.07$ fm, $\beta \sim 6.2$ systematic effects related to a proper identification of the topological background are negligible at these couplings.

We adopt cooling to extract Q (the gradient (or Wilson) flow gives, configuration by configuration, equivalent results, see C. Bonati, M.D., arXiv:1401.2441)

Severeness of the sign problem





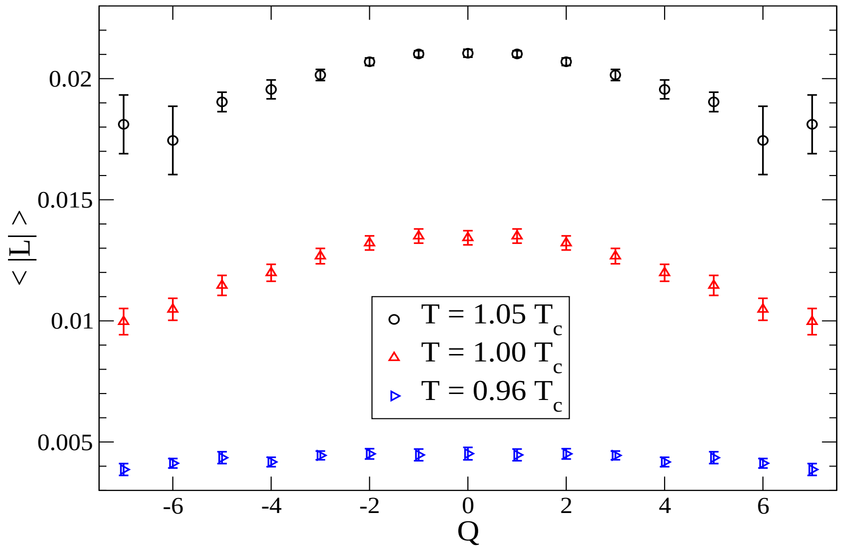
LEFT: **average phase for different θ and cooling times at $T \sim 1.06\, T_c$. Q.**

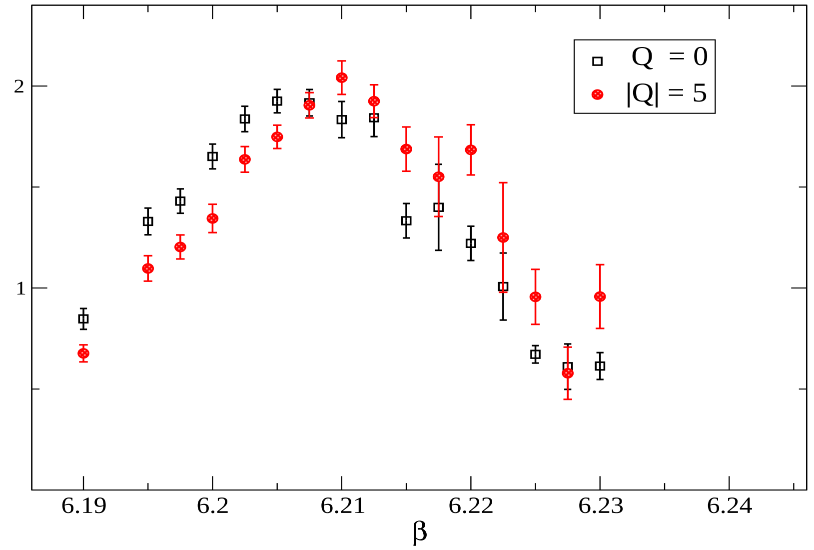
RIGHT: **average phase as a function of θ for different temperatures**

The average phase decays rapidly and one barely reaches, on this lattice size, θ equal to a small fraction of π.

The situation changes rapidly across T_c and looks better at high T, where the topological activity is suppressed.

Dependence of observables on the topological sector





LEFT: Polyakov loop modulus as a function of the topological sector Q.

RIGHT: Polyakov loop susceptibility in different topological sectors

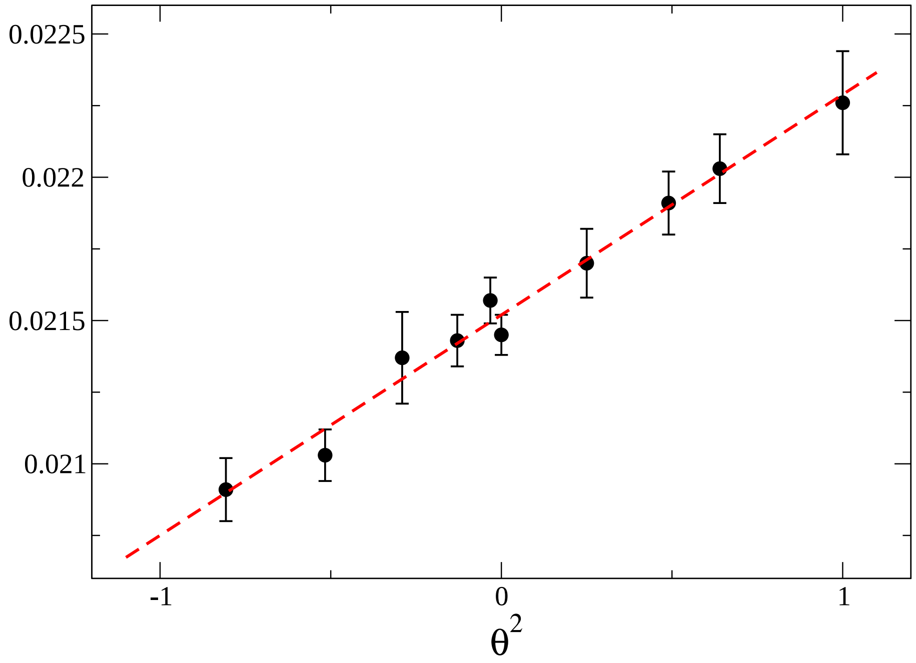
A non-trivial dependence on θ implies a non-trivial dependence on the topological sector Q.

This is clearly visible above, even T_c seems to depend on Q.

WARNING for simulations performed at fixed topological sector.

Analytic continuation vs. Reweighting

Average Polyakov loop at $T \simeq 1.055\, T_c$

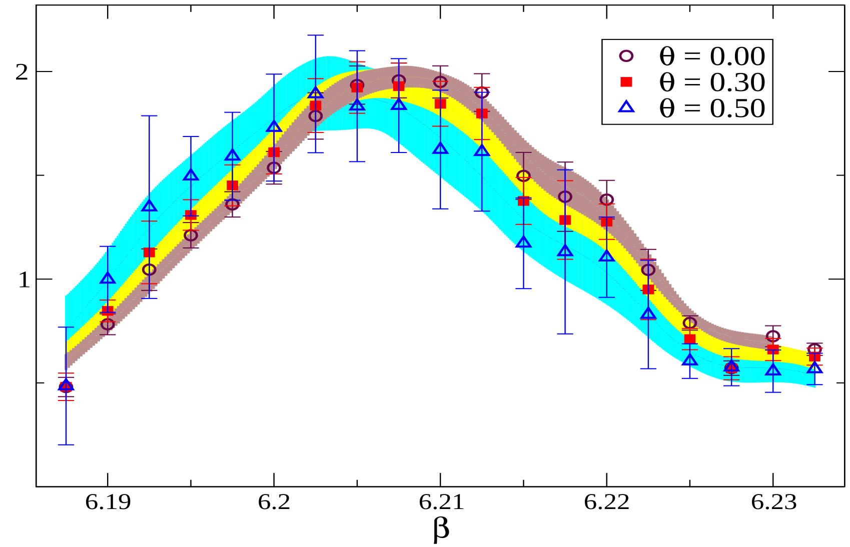


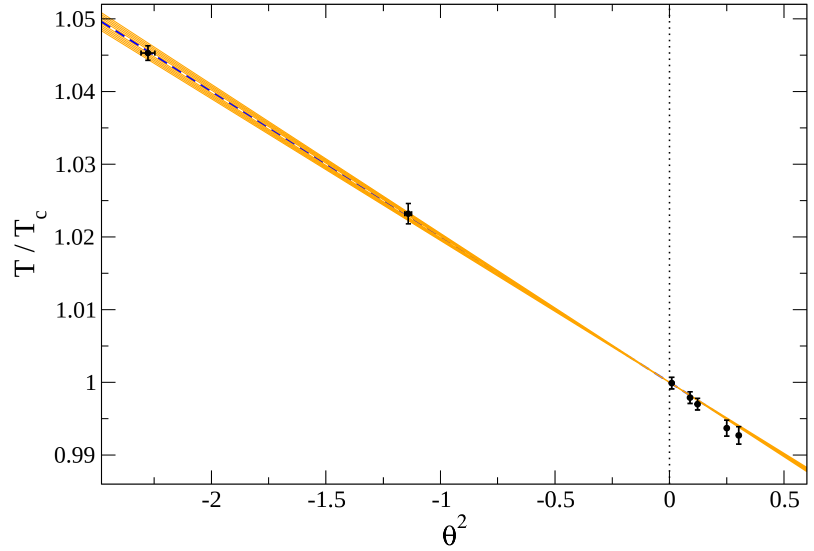
Results at imaginary and real θ (negative or positive θ^2) are perfectly compatible with each other.

Notice that results at real θ are completely correlated to each other (reweighting from the same $\theta = 0$ ensemble).

Analytic continuation vs. Reweighting

Location of T_c





LEFT: **Polyakov loop susceptibility for different real $\theta\ Q$.**

RIGHT: **Critical temperature estimate: extrapolation from imaginary θ compared to reweighting.**

Results from reweighting are compatible with those from analytic continuation

4 – Sketching the $T-\theta$ phase diagram

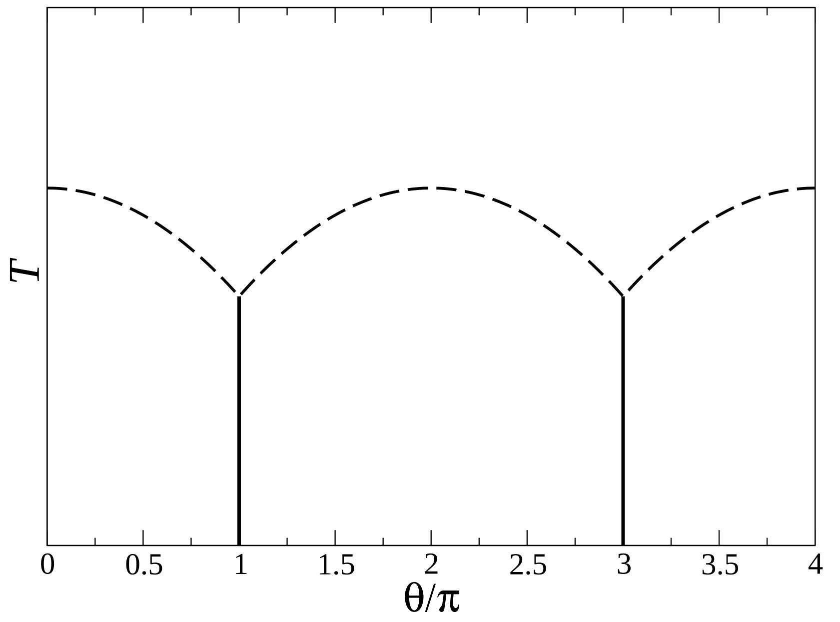
M. D. and F. Negro, PRD 88, 034503 (2013)

Approximate solution to the sign problem permit a reliable study in a limited region around $\theta = 0$. As for the whole phase structure in the $T-\theta$ plane, we can only make a reasonable guess, based on the following considerations.

- **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 (C. Bonati, M. D., H. Panagopoulos and E. Vicari, PRL 110, 252003 (2013) 1301.7640). 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**

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

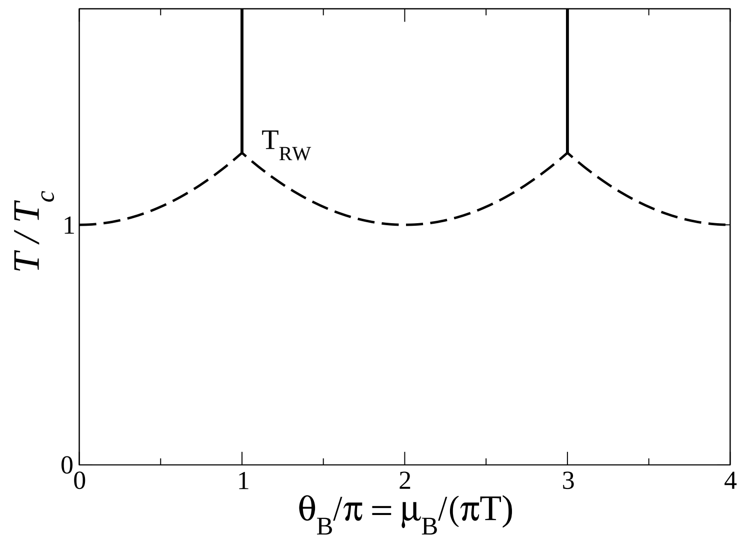
This is the resulting conjectured phase diagram

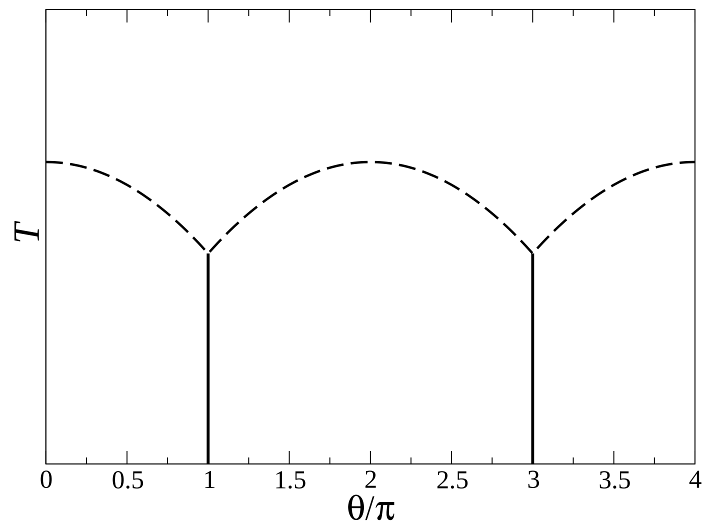


There is, actually, a further unjustified assumption: the critical line $T_c(\theta)$ touches the low-T transition present at $\theta = \pi$ exactly at its endpoint.

This is just a personal bias, the two lines could cross or even do not touch at all ...

A striking dual-similarity ($T \to 1/T$) emerges with the phase diagram at imaginary μ_B





- 2π **periodicity in** $Im(\mu_B)/T$ **is smoothly realized at low** T**, but phase transitions (Roberge-Weiss lines) present at high** T **for odd multiples of** π**. This is related to the relevant degrees of freedom carrying baryon charge 1 below** T_c **and** $1/N_c$ **above** T_c**.**

- **Can we then interpret that objects with integer** Q **dominate the high** T **regime (instantons, calorons), and fractionally charged objects dominate the low** T **regime (instanton quarks? monopoles?)? Does that give a hint about the relevant degrees of freedom for confinement?**

5 – Conclusions

- **We have explored the small θ region of the $T-\theta$ phase diagram in $SU(3)$ pure gauge theory, obtaining consistent results by analytic continuation and by reweighting.**

- **T_c decreases with θ, with a quadratic coefficient of order $1/N_c^2$.**

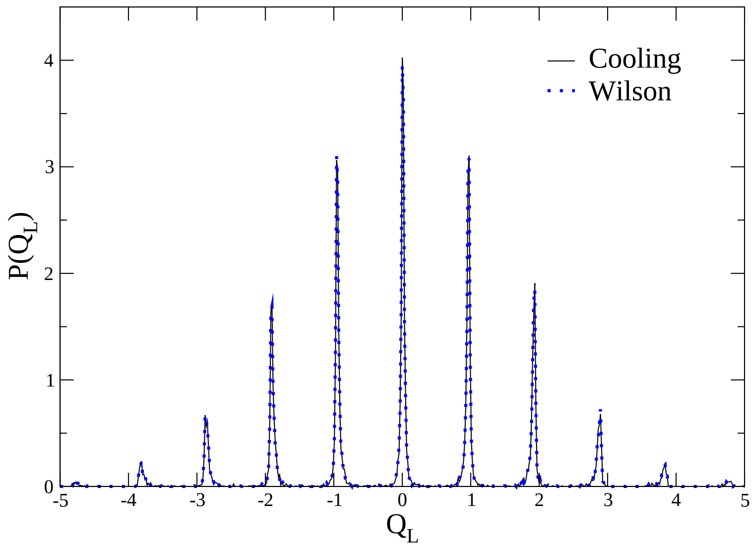
$$T_c(\theta)/T_c(0) = 1 - R_\theta\,\theta^2 + O(\theta^4) \qquad\qquad R_\theta = 0.0178(5) \text{ for } SU(3)$$

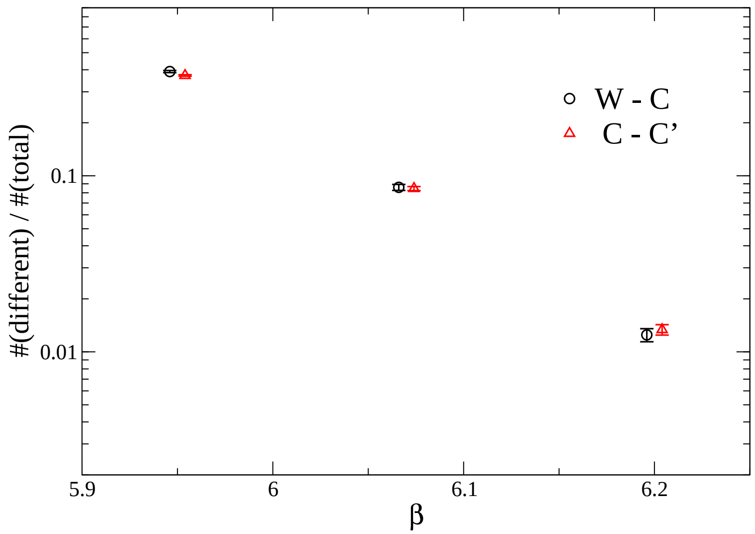
- **We have made some speculations about the whole phase structure in the $T-\theta$ plane and a possible striking dual-similarity with the phase diagram at imaginary baryon chemical potential.**

- **For people trying to solve the sign problem completely: there are lot of interesting things to be studied at $\theta \neq 0$, maybe in a simpler context (pure gauge theory).**

BACKUP SLIDES

Comparison of cooling and the gradient (Wilson) flow





LEFT Probability distribution of the topological charge for $\beta = 6.2$, evaluated after 21 cooling steps and after Wilson flow with $\tau = 7$ (correspondence by matching plaquette values) on a 20^4 lattice. The two distributions are hardly distinguishable.

RIGHT Fraction of configurations where different methods give different topological charges. Circles refer to the comparison between cooling and Wilson flow, while triangles refer to different cooling implementations. Data points have been slightly shifted horizontally in order to distinguish them.

Average topological charge at imaginary θ: continuum limit

from H. Panagopoulos and E. Vicari, JHEP 1111, 119 (2011) 1109.6815