$\theta$-dependence of the deconfinement temperature in Yang-Mills theories

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Sign Problem in QCD and Beyond

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INFN
1) Introduction to the problem.

2) Topological $\theta$-term and sign problem.

3) The lattice discretization.

4) Numerical results from LGT.

5) Large $N_c$ estimate.

6) Conclusions.
SU(3) gauge theory phase diagram in the $T - \theta$ plane.

Does $T_c$ depend on $\theta$? Is it growing or decreasing?
1) Introduction.

Our aim:
1) Study if and how the deconfinement transition temperature depends on the topological $\theta$-term.

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

2) Perform a large-$N_c$ estimation of this dependence.

3) Compare these calculations.
2) Topological $\theta$-term and sign problem.

We consider the following continuum action in euclidean metric:

$$S = S_{YM} + S_\theta$$

The pure gauge term:

$$S_{YM} = -\frac{1}{4} \int d^4x \; F_{\mu\nu}^a(x)F_{\mu\nu}^a(x)$$

and the topological $\theta$-term:

$$S_\theta = -i\theta \frac{g_0^2}{64\pi^2} \int d^4x \; \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x)F_{\rho\sigma}^a(x) \equiv -i\theta \int d^4x \; q(x) \equiv -i\theta Q[A]$$
2) Topological $\theta$-term and sign problem.

LGT techniques are based on the possibility to interpret the partition function integrand

$$ Z(T, \theta) = \int D[A] \ e^{-S_{YM} + i\theta Q[A]} $$

as a probability distribution for the fields $A^a_\mu$.

But it is complex! Bad news... sign problem!

Anyhow LGT are preferred ways to probe the non-perturbative properties of YM theories.
Can we somehow re-arrange things so that we can apply LGT techniques to such a model?
2) Topological $\theta$-term and sign problem.

Via an imaginary $\theta = i \theta_I$ term we can "solve" the sign problem.

[Azcoiti et al., PRL 2002; Alles and Papa, PRD 2008; Horsley et al., arxiv:0808.1428 [hep-lat]; Panagopoulos and Vicari, JHEP 2011]

Analyticity around $\theta = 0$ is supported by the current knowledge of the vacuum free energy derivatives with respect to $\theta$ evaluated at $\theta = 0$.

[Alles, D’Elia and Di Giacomo, PRD 2005; Vicari and Panagopoulos, Physics Reports 2008]

Studying the dependence on $\theta_I$ we will have access to a (small) range of real $\theta$ via analytic continuation.

The continuum partition function to be put on the lattice is:

$$Z(T, \theta) = \int D[A] \ e^{-S_{YM} - \theta_I Q[A]}$$
3) The lattice discretization.

The topological charge operator can be discretized as:

\[ Q_L[U] = \frac{-1}{2^9 \pi^2} \sum \text{Lattice} \sum_{n} \sum_{\mu \nu \rho \sigma = \pm 1} \tilde{\epsilon}_{\mu \nu \rho \sigma} \text{Tr} (\Pi_{\mu \nu}(n) \Pi_{\rho \sigma}(n)) \]

Using the Wilson action for \( S_{YM} \) the lattice partition function is:

\[
Z(T, \theta) = \int D[U] e^{-S_{YM}^L[U] - \theta L Q_L[U]}
\]

Due to a finite multiplicative renormalization \( Q_L \) is related to the integer valued \( Q \) by:

\[ Q_L = Z(\beta) Q + O(a^2) \]

[Campostrini, Di Giacomo and Panagopoulos, Phys Lett B 1988]

So the \( \theta \)-term is also

\[ S_\theta \equiv -\theta_L Q_L = -\theta_L Z(\beta) Q = -\theta I Q \]

Francesco Negro  \( \theta \)-dependence of deconfinement temperature in YM theories
3) The lattice discretization.

In this simple action each link appears *linearly*.

\[ \Downarrow \]

We can exploit *standard* Heatbath and Overrelaxation algorithms.

It is necessary to modify the staples definition. Pictorially:

With more complicated topological charge definitions on the lattice such standard algorithms wouldn’t have been applicable.
\( \mathbb{Z}_3 \) center symmetry holds also when we introduce the topological term in the action.

Deconfinement \( \rightarrow \) spontaneous breaking of \( \mathbb{Z}_3 \) center symmetry.

Order parameter: Polyakov loop

\[
L(\beta, \theta_L) = \langle L \rangle_{\beta, \theta_L} = \left\langle \frac{1}{V_s} \sum_{n_x,n_y,n_z} \text{Tr} \left( \prod_{i=0}^{N_t-1} U_t(n_x, n_y, n_z, i) \right) \right\rangle_{\beta, \theta_L}
\]

At a fixed \( \theta_L \) we find the transition in correspondence of the susceptibility peak:

\[
\chi_L(\beta, \theta_L) = V_s \left( \langle L^2 \rangle_{\beta, \theta_L} - \langle L \rangle_{\beta, \theta_L}^2 \right)
\]
4) Numerical results from LGT: ingredients for $R_\theta$.

1) $Z(\beta)$ in order to determine $\theta_I = Z(\beta)\theta_L$.

Compute $Q_L$ via the operator previously defined.
Compute $Q$ via cooling algorithm.
Evaluate:

$$Z(\beta) = \frac{\langle Q_L Q \rangle_\beta}{\langle Q^2 \rangle_\beta}$$

as proposed in [Panagopoulos and Vicari, JHEP 2011]

Simulations were performed on a symmetric $16^4$ lattice for 8 values of $\beta$ spanning in $5.7 - 6.3$.
The results were checked for some $\beta$ on a symmetric $24^4$ lattice.
4) Numerical results from LGT: ingredients for $R_\theta$.

2) $\beta_c(\theta_I)$ in order to measure $T_c(\theta_I)/T_c(0)$.
For various $\theta_L$ we search $\beta_c$ via a Lorentzian fit.
Using the non-perturbative determination of $a(\beta)$ in [Boyd et al., Nucl Phys B 1996] we have:

$$\frac{T_c(\theta_I)}{T_c(0)} = \frac{a(\beta_c(\theta = 0))}{a(\beta_c(\theta_I))}$$

Where $\theta_I = Z(\beta_c)\theta_L$.
Simulations have been performed for various lattice spacings in order to approach the continuum limit.
We choose $a \simeq 1/(4T_c(0))$, $a \simeq 1/(6T_c(0))$ and $a \simeq 1/(8T_c(0))$.
The lattices we have used are $16^3 \times 4$, $24^3 \times 6$ and $32^3 \times 8$. 
4) Numerical results from LGT: Cooling.

Topological charge of a config: cooling + scaling + rounding.
Example for $16^4$ at $\beta = 5.90$: 

![Histogram of "hot" topological charge](image)
4) Numerical results from LGT: Cooling.

Topological charge of a config: cooling + scaling + rounding.
Example for $16^4$ at $\beta = 5.90$:
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Topological charge of a config: cooling + scaling + rounding. Example for $16^4$ at $\beta = 5.90$:
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Topological charge of a config: cooling + scaling + rounding.
Example for $16^4$ at $\beta = 5.90$:
4) Numerical results from LGT: $Z(\beta)$.

Simulation on $16^4$ lattice and polynomial cubic interpolation.
4) Numerical results from LGT: $\beta_c(\theta_I)$.

Determination of $\beta_c$ e.g. on the $24^3 \times 6$ lattice. $L$ and $\chi_L$ data and $\beta$-reweighting analysis.

Weak increase in $\chi_L$ peak.

Stronger transition?
4) Numerical results from LGT: $\beta_c(\theta_I)$.

<table>
<thead>
<tr>
<th>lattice</th>
<th>$\theta_L$</th>
<th>$\beta_c$</th>
<th>$\theta_I$</th>
<th>$T_c(\theta_I)/T_c(0)$</th>
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<td>$16^3 \times 4$</td>
<td>0</td>
<td>5.6911(4)</td>
<td>0</td>
<td>1</td>
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<tr>
<td>$16^3 \times 4$</td>
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<td>0.370(10)</td>
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<td>0.747(15)</td>
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<td>1</td>
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<tr>
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<td>0.5705(60)</td>
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<tr>
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</tbody>
</table>

$\theta_I$ values spanning in $[0; 2.5]$

Typical statistics for each size and for each $\theta_L$:

$\sim 10^5 - 10^6$
4) Numerical results from LGT: $R_\theta$.

We find:

- $R_{\theta}^{N_t=4} = 0.0299(7)$
- $\chi^2/d.o.f. \sim 0.3$

- $R_{\theta}^{N_t=6} = 0.0235(5)$
- $\chi^2/d.o.f. \sim 1.6$

- $R_{\theta}^{N_t=8} = 0.0204(5)$
- $\chi^2/d.o.f. \sim 0.7$

$T_c$ increases for imaginary coupling then, by analytic continuation, it decreases for real $\theta$. 
4) Numerical results from LGT: continuum extrapolation.

Assuming quadratic finite lattice spacing corrections to $R_\theta$:

$$ R^{N_t}_\theta = R^{\text{cont}}_\theta + c/N_t^2 $$

we can extrapolate to the continuum limit to get

$$ R^{\text{cont}}_\theta = 0.0175(7) \text{ with } \chi^2/d.o.f. \sim 1 $$
4) Numerical results from LGT: continuum extrapolation.

Preliminary finer lattice spacing: for \( N_t = 10 \) we found
\[
R_{\theta}^{N_t=10} = 0.0190(9)
\]
Extrapolation towards the continuum limit leads to:
\[
R_{\theta}^{\text{cont}} = 0.0174(5) \quad \text{with } \chi^2/d.o.f. \sim 0.7
\]
5) Large $N_c$ estimate.

**1\textsuperscript{st}-order transition** $\rightarrow$ 

2 phases with different free energy densities crossing at $T_c$.

\[
f_c(T_c) = f_d(T_c) \\
 f'_c(T_c) \neq f'_d(T_c)
\]

Close to $T_c$ and using $t = (T - T_c)/T_c$ the free energies are:

\[
\frac{f_c(t)}{T} = A_c t + O(t^2) \\
\frac{f_d(t)}{T} = A_d t + O(t^2)
\]

From the usual relations:

\[
Z = e^{-\frac{V_s f(T)}{T}} \\
\epsilon(T) = \frac{T^2}{V_s} \partial_T \log Z
\]

we easily find that the slope difference is related to the latent heat

\[
\Delta \epsilon = \epsilon_d(T_c) - \epsilon_c(T_c) = T_c(A_c - A_d)
\]
5) Large $N_c$ estimate.

When we have $\theta \neq 0$ the free energy density is modified by

$$f(T, \theta) = f(T, \theta = 0) + \frac{\chi(T)\theta^2}{2} + O(\theta^4)$$

In the large $N_c$ limit $\chi(T)$ is a step function:

$$\chi(T < T_c) = \chi(T = 0) \equiv \chi \neq 0 \quad \chi(T > T_c) = 0$$

[Alles, D’Elia and Di Giacomo, Phys Lett B ’96-'97-'00; Del Debbio, Vicari and Panagopoulos, JHEP 2004; Lucini, Teper and Wenger, Nucl Phys B 2005]

This modifies the free energies in:

$$\frac{f_c(t)}{T} = A_c t + \frac{\chi \theta^2}{2T} \quad \frac{f_d(t)}{T} = A_d t$$

$T_c$ is found when $f_c = f_d \rightarrow \frac{T_c(\theta)}{T_c(0)} = 1 - \frac{\chi}{2\Delta \epsilon} \theta^2$
5) **Large $N_c$ estimate.**

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This modifies the free energies in:

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$T_c$ is found when $f_c = f_d \rightarrow \frac{T_c(\theta)}{T_c(0)} = 1 - R_\theta^\text{large } N_c \theta^2$
5) Large $N_c$ estimate.

From the large $N_c$ estimates in [Lucini, Teper and Wenger, JHEP 2005]:

\[
\frac{\chi}{\sigma^2} = 0.0221(14) \quad \frac{\Delta\epsilon}{N_c^2 T_c^4} = 0.344(72) \quad \frac{T_c}{\sqrt{\sigma}} = 0.5978(38)
\]

we can evaluate $R^{\text{large } N_c}_\theta$:

\[
R^{\text{large } N_c}_\theta = \frac{\chi}{2\Delta\epsilon} = \frac{0.253(56)}{N_c^2} + O\left(\frac{1}{N_c^4}\right)
\]

The argument in [Witten, PRL 1998] supports this dependence on $N_c$. Large-$N_c$ limit $\rightarrow$ expansion variable $\frac{\theta}{N_c} \rightarrow R_\theta\theta^2 \rightarrow R_\theta \propto \frac{1}{N_c^2}$

Let’s recall both our results and compare them in the case $N_c = 3$.

\[
R^{\text{cont}}_\theta = 0.0175(7) \quad R^{\text{large } N_c}_\theta (N_c = 3) = 0.0281(62)
\]
6) Conclusions

- Use of imaginary $\theta_I$ parameter to cure sign problem for LGT.
- Deconfinement transition temperature dependence on $\theta_I$.
- Determination of the quadratic coefficient $R_{\theta}^{\text{cont}}$.
- Large $N_c$ estimate and comparison.

Perspectives:
- Finer lattice spacings to improve continuum limit approach. ✓
- Weaker transition? Finite size scaling study.
- Extend the analysis to $SU(2)$ and $SU(4)$.
- Reweighting for real $\theta$ starting from $\theta = 0$. ✓
7) Backup: conjectured phase diagram.

At least in the large $N_c$ limit when only $O((\theta/N_c)^2)$ terms are relevant we can suppose the phase diagram to show $2\pi$-periodicity and cusps in $\theta = (2k + 1)\pi$. 

\begin{figure}
\centering
\includegraphics[width=\textwidth]{phase_diagram.png}
\caption{\textit{\(\theta\)-dependence of deconfinement temperature in YM theories}}
\end{figure}
7) Backup: Correlation between $Q$ and $L$.

If we imagine to reweight in $\theta$ for the Polyakov loop $L$

$$
\langle L \rangle_\theta = \frac{\langle Le^{i\theta Q} \rangle_{\theta=0}}{\langle e^{i\theta Q} \rangle_{\theta=0}} = \frac{\sum_Q L(Q) p(Q) e^{i\theta Q}}{\sum_Q p(Q) e^{i\theta Q}}
$$

we realize that $\langle L \rangle_\theta$ can depend on $\theta$ only if $L$ depends on $Q$: actually $\theta$ and $Q$ are conjugated variables.

We expect $L$ to depend on $Q$: true in the coarsest lattice ($N_t = 4$) if away from the thermodynamic limit (e.g. $N_s = 16$).

Study the transition in different sectors to look for possible $T_c$ dependence on $Q$. 

Francesco Negro \hspace{1cm} $\theta$-dependence of deconfinement temperature in YM theories
7) Backup: Correlation between Q and L.
Dependence of $Q$ on $\beta$ on a $40^3 \times 10$ lattice at two values of $\theta_I$. 

\[ \text{Theta}_L = 8.4 \rightarrow \text{Theta}_I = 1.51 \]
\[ \text{Theta}_L = 13.4 \rightarrow \text{Theta}_I = 2.46 \]
7) Backup: move along $\theta_I = \text{const}$

Reweighting analysis on all $16^3 \times 4$ data.

We obtain a 3D plot for the polyakov loop susceptibility:
7) Backup: move along $\theta_I = \text{const}$

Moving along constant $\theta_I$ instead of constant $\theta_L$.
For $\theta_I \simeq 0.37$ and $\theta_L = 5.0$
7) Backup: move along $\theta_I = \text{const}$

Moving along constant $\theta_I$ instead of constant $\theta_L$.
For $\theta_I \simeq 1.14$ and $\theta_L = 15.0$
Moving along constant $\theta_I$ instead of constant $\theta_L$.
For $\theta_I \simeq 2.04$ and $\theta_L = 25.0$.