$\Theta$ dependence and large $N$

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Overview of results on the $\theta$ dependence of 4D $SU(N)$ gauge theories, for $N = 3$ and in the large-$N$ limit.

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4D $SU(N)$ gauge theories have a nontrivial $\theta$ dependence

$$\mathcal{L}_\theta = \frac{1}{4} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x) - i\theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x),$$

$q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x)$ is the topological charge density. $\theta$ is a parameter of the strong interactions, which violates parity and time reversal symmetry.

$|\theta| \lesssim 10^{-10}$ from experimental bounds on the electric dipole moment of the neutron, $d_n \sim \theta e m^2_\pi / m_n^3 \approx 10^{-16} \theta e$ cm.

Nevertheless $\theta$ dependence remains a physically interesting issue in 4D $SU(N)$ gauge theories. For example, it is related to $U(1)_A$ problem.
In the semiclassical picture, instantons give rise to tunneling between different $n$-vacua, leading to $\theta$ vacua: $|\theta\rangle = \sum_n e^{in\theta} |n\rangle$, whose ground-state energy is given by $F(\theta) = -\frac{1}{V} \ln \int [dA] \exp(- \int d^4 x \mathcal{L}_\theta)$, where the $\theta$ dependence vanishes in perturbation theory: its study requires nonperturbative approaches.

First approaches employed effective chiral Lagrangians:

$$\mathcal{L}_{\text{ch}} = \frac{1}{4} F^2 \text{Tr}[\partial_\mu U^\dagger \partial_\mu U] - \frac{1}{2} \sum \text{Tr}[M e^{i\theta/N_f} U^\dagger + M^\dagger e^{-i\theta/N_f} U]$$

from which $\chi \equiv \partial F(\theta)/\partial \theta^2 |_{\theta=0} = -m_f \langle \bar{\psi}\psi \rangle / N_f^2$.

A robust numerical evidence of a nontrivial $\theta$ dependence has been provided by MC simulations of the lattice formulation of the theory.
Plan of the talk:

- Large-$N$ framework and $U(1)_A$ problem
- Ground-state energy and its expansion around $\theta = 0$
- $N$-scaling behavior by large-$N$ arguments
- Lattice formulation and results from MC simulations
  - topological susceptibility for $SU(3)$ and large $N$
  - $O(\theta^4)$ term of the expansion
  - $\theta$ dependence of the spectrum
  - $\theta$ dependence at finite temperature
- $\theta$ dependence in 2D $CP^{N-1}$ models

The large-$N$ limit, $N \to \infty$ keeping $g^2N, N_f$ fixed, is a very useful framework to investigate the physics of strong interactions: the phenomenology of QCD in the large-$N$ limit presents remarkable analogies with that of the real world.

The leading large-$N$ contributions come from planar diagrams, each fermion loop introduces a factor $1/N$.

The large-$N$ solution of 4D $SU(N)$ gauge theories is still unknown, and therefore it is not possible to perform a systematic $1/N$ expansion. The problems in determining the large-$N$ saddle point are essentially related to the matrix nature of the theory. Nevertheless, large-$N$ arguments lead to several nontrivial predictions.

The $1/N$ expansion has been instead successfully developed in vector models, such as $O(N)$-symmetric theories and $CP^{N-1}$ models.
The $\theta$ dependence is relevant for the hadronic physics, an example is the solution of the $U(1)_A$ problem, i.e. the missing evidence of the $U(1)_A$ symmetry in the QCD spectrum.

The existence of nontrivial topological configurations, contributing to the matrix elements of the anomaly, $\partial_\mu j_5^\mu(x) = i2N_f q(x)$, gives rise to a nonconservation of the $U(1)_A$ charge.

**Within the large-$N$ framework:** nontrivial $\theta$ dependence at a nonperturbative level, at the leading planar level of the $1/N$ expansion. But massless quarks, whose contribution is subleading at large-$N$, make $\theta$ dependence disappear in the massless limit.

This apparent contradiction is solved by the presence of a particle with $m_s^2 = O(1/N)$, having the same quantum numbers of $Q$, and therefore related to the lightest flavor-singlet pseudoscalar in nature, i.e. the $\eta'$. 
Further developments of these ideas led to the Witten-Veneziano relations:

\[
\chi = \frac{f_s^2 m_s^2}{4N_f}, \quad \text{or} \quad \frac{4N_f}{f_\pi^2} \chi = m_{\eta'}^2 + m_\eta^2 - 2m_K^2,
\]

\[
\chi = \frac{\partial F(\theta)}{\partial \theta^2}|_{\theta=0} = \int d^4 x \langle q(x)q(0) \rangle = \frac{\langle Q^2 \rangle}{V}
\]

By substituting \( N_f = 3 \) and the experimental values \( f_\pi \approx 131 \text{ MeV} \), \( m_{\eta'} \approx 958 \text{ MeV} \), \( m_\eta \approx 547 \text{ MeV} \), \( m_K \approx 494 \text{ MeV} \), \( \chi \approx (180 \text{ MeV})^4 \)

\( \chi \) should be considered that of the pure gauge theory, due to its large-\( N \) derivation. This makes its check within the lattice formulation much easier.
Let us introduce $f(\theta) = (F(\theta) - F(0))/\sigma^2$ \((\sigma \equiv \text{string tension})\), where $F(\theta) = -\frac{1}{V} \ln \int [dA] \exp(-\int d^4x \mathcal{L}_\theta)$, and parametrize it as

$$f(\theta) = \frac{1}{2} C \theta^2 s(\theta),$$

with $s(0) = 1$, $C = \chi/\sigma^2$, $\chi \equiv \partial^2 F(\theta)/\partial \theta^2|_{\theta=0}$.

$s(\theta)$ can be expanded as $s(\theta) = 1 + b_2 \theta^2 + b_4 \theta^4 + \cdots$, whose coefficients can be related to the zero-momentum $n$-point connected correlation functions of the topological charge density $q(x)$, e.g.,

$$b_2 = -\chi_4/(12\chi) \quad \text{and} \quad \chi_4 = \int d^4x_1 d^4x_2 d^4x_3 \langle q(0)q(x_1)q(x_2)q(x_3) \rangle|_{\theta=0}$$

Correlation functions involving zero-momentum insertions of $q(x)$ can be defined in a nonambiguous way \((\text{Lüscher, 2004})\), and therefore the coefficients $b_{2n}$ are well defined RG invariant quantities $b_{2n}$ parametrize the deviations from a Gaussian distribution,

$$P(Q) = \frac{1}{\sqrt{2\pi\langle Q^2 \rangle}} \exp\left(-\frac{Q^2}{2\langle Q^2 \rangle}\right),$$

of the topological charge.
\( \theta \) dependence of the spectrum

\[ \sigma(\theta) = \sigma \left( 1 + s_2 \theta^2 + ... \right), \] where \( \sigma \) is the string tension at \( \theta = 0 \).

Similarly for the lowest glueball state:

\[ M(\theta) = M \left( 1 + g_2 \theta^2 + ... \right), \] where \( M \) is the \( 0^{++} \) glueball mass at \( \theta = 0 \). At \( \theta \neq 0 \), the lightest glueball state does not have a definite parity anymore, but it becomes a mixed state of \( 0^{++} \) and \( 0^{-+} \) glueballs.

The coefficients of the above expansions can be computed from appropriate correlators at \( \theta = 0 \).
Large-$N$ scaling arguments applied to 
\[ \mathcal{L}_\theta = \frac{1}{4} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x) - i \theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x) \] indicate that the relevant scaling variable in the large-$N$ limit is $\bar{\theta} \equiv \theta/N$.

The Lagrangian is $O(N^2)$ and the large-$N$ limit is performed keeping $g^2 N$ fixed.

\[ f(\theta) \equiv (F(\theta) - F(0))/\sigma^2 = \frac{1}{2} C \theta^2 (1 + b_2 \theta^2 + b_4 \theta^4 + ...) = N^2 \bar{f}(\bar{\theta}) \]

$\bar{f}(\bar{\theta})$ has a nontrivial large-$N$ limit:

\[ \frac{1}{2} C_\infty \bar{\theta}^2 (1 + \bar{b}_2 \bar{\theta}^2 + \bar{b}_4 \bar{\theta}^4 + \cdots), \]

where $C \equiv \chi/\sigma^2 = C_\infty + c_2/N^2 + \ldots$, and $b_{2j} = \bar{b}_{2j}/N^{2j} + \ldots$.

Analogously, the $\theta$-dependence of the lowest glueball mass can be written as 
\[ M(\theta)/M(\theta = 0) = 1 + g_2 \theta^2 + \ldots = \mathcal{M}(\theta), \]
where $\mathcal{M}(\theta) \to 1 + \bar{g}_2 \bar{\theta}^2 + \ldots$ in the large-$N$ limit, thus $g_{2j} = \bar{g}_{2j}/N^{2j} + \ldots$. 
The large-$N$ scaling behavior is apparently incompatible with the periodicity condition $f(\theta) = f(\theta + 2\pi)$, which is a consequence of the quantization of the topological charge. Indeed a regular function of $\bar{\theta} = \theta/N$ cannot be invariant for $\theta \rightarrow \theta + 2\pi$, unless it is constant.

Witten conjecture: the ground-state energy $F(\theta)$ in the large-$N$ limit is a multibranched function because of many candidate vacuum states which all become stable, although not degenerate, for $N = \infty$.

$F(\theta) - F(0) = A \text{Min}_k (\theta + 2\pi k)^2 + O(1/N)$, in particular, for sufficiently small values of $\theta$, i.e. $|\theta| < \pi$, $F(\theta) - F(0) = A \theta^2 + O(1/N^2)$
The study of $\theta$ dependence requires a nonpertubative approach: Wilson lattice formulation of QCD, from the critical continuum limit of a 4D statistical system:

$$Z = \int [dU] \exp(-S_L),$$

$$S_L = -(2/g_0^2)a^4 \sum \text{ReTr} [U_\mu(x)U_\nu(x + a\hat{\mu})U^\dagger_\mu(x + a\hat{\nu})U^\dagger_\nu(x)],$$

where $U_{\mu,\nu}$ are $SU(N)$ matrix variables defined on the bonds of a 4D lattice. Formally, in the $a \to 0$ limit, one recovers $S = \int d^4x \frac{1}{2g_0^2} \text{Tr} F_{\mu\nu}F_{\mu\nu}$.

The statistical theory develops a mass gap, and therefore a length scale $\xi$. The continuum theory is defined in the critical limit $g_0^2 \to 0$, when $\xi \to \infty$:

$$\xi = a \exp \int g_0^0 dg/\beta_L(g) \sim a(b_0g_0^2)^{-b_1/2b_2} \exp[1/(2b_0g_0^2)],$$

where

$$\beta_L = adg_0/da = -b_0g_0^3 - b_1g_0^5 + ...$$

The lattice formulation lends itself to statistical mechanics techniques, such as MC simulations.
The complex nature of the $\theta$ term in the Euclidean QCD Lagrangian prohibits a direct MC simulation at $\theta \neq 0$.

Information on the $\theta$ dependence of physically relevant quantities can be obtained by computing their expansion around $\theta = 0$:

$$f(\theta) \equiv (F(\theta) - F(0))/\sigma^2 = \frac{1}{2}C\theta^2(1 + b_2\theta^2 + b_4\theta^4 + \ldots)$$

The coefficients $C$ and $b_{2n}$ of such an expansion can be determined from appropriate correlation functions with insertions of $q(x)$ at $\theta = 0$, such as $\langle q(x_1)q(x_2)\ldots q(x_{2n}) \rangle$.
Topology relies on certain smoothness assumptions, however the path integral requires integration over all configurations.

The lattice regularization makes the topology strictly trivial, because its configuration space is simply connected. The physical topological properties are expected to be recovered in the continuum limit.

**Straightforward approach:** discretization of $q(x)$ to obtain a corresponding lattice operator $q_L(x) \longrightarrow a^4 q(x) + O(a^6)$. For example, $q_L(x) = -\frac{1}{2^4 \times 32\pi^2} \sum_{\mu\nu\rho\sigma=\pm 1}^\pm \epsilon_{\mu\nu\rho\sigma} \text{Tr} [\Pi_{\mu\nu} \Pi_{\rho\sigma}]$

But at a quantum level: $q_L(x) \longrightarrow a^4 Z_L(g_0^2) q(x) + O(a^6)$. $q(x)$ is a RG invariant operator, thus $Z_L(g_0)$ is a finite function.

This straightforward approach allows us to compute correlation functions of $q(x)$, $G_q^{(n)}(x_1, x_2, ... x_n) = a^{-nd} Z_L(g_0)^{-n} \langle q_L(x_1) q_L(x_2) ... q_L(x_n) \rangle + O(a)$ when $x_i \neq x_j$ for any $i \neq j$. The coincidence of points gives rise to contact terms, which make the relation between lattice and continuum correlation functions complicated.
The $\theta$ dependence of the ground-state around $\theta = 0$ involves also correlations at coincident points, i.e. in the limit $|x_i - x_j| \to 0$. In particular, $\chi = \int d^4x \langle q(0)q(x) \rangle$

The lattice counterpart $\langle q_L(x)q_L(y) \rangle$ does not reconstruct correctly the singular behavior for $x \to y$, giving rise to dominant unphysical contributions in the continuum limit.

**Geometrical, smoothing and off-equilibrium** techniques have been used to address this problem. They rely on heuristic arguments, and their systematic errors are not under robust theoretical control. However, several numerical checks and comparisons have shown that they provide quite accurate results.

Substantial progress with the **fermionic definition** through the index of the overlap Dirac operator (or any Dirac operator satisfying GW relation), \( q_i(x) = \frac{1}{2} \text{Tr}[\gamma_5 D(x, x)] \), provides a well–defined estimator for $Q$, but at a much higher computational cost.
SU(3) results for $\chi$, from many numerical works ... Overall consistency among the methods. Most recent results suggest $\chi/\sigma^2 = 0.028(2)$, and $\chi r_0^4 = 0.057(5)$ [$\sigma^{1/2} r_0 = 1.19(1)$]

**Agreement with the Witten-Veneziano relations.**

$\chi = f_{\eta'}^2 m_{\eta'}^2 / 4N_f$ gives $\chi^{1/4} \approx 190$ MeV using the actual values of $f_\pi$, $m_{\eta'}$, and $N_f = 3$; from the refined relationship

$$(4N_f / f_\pi^2) \chi = m_{\eta'}^2 + m_{\eta}^2 - 2m_K^2 \rightarrow \chi^{1/4} \approx 180 \text{ MeV}$$

Then, using the quite standard values $\sqrt{\sigma} = 440$ MeV and $r_0 = 0.5$ fm, we obtain $\chi^{1/4} = 180(3)$ MeV and $\chi^{1/4} = 193(4)$ MeV respectively, the difference is related to the uncertainty in the physical scale for $\sigma$ and $r_0$. 
The large-$N$ limit of \( C \equiv \partial^2 f(\theta)/\partial \theta^2 = \chi/\sigma^2 \)

The large-$N$ limit can be investigated numerically, by performing MC simulations for various values of $N$, and checking the convergence to $N = \infty$ with the expected $1/N^2$ approach.

Results from works of Lucini, Teper, Del Debbio, Panagopoulos, V., Giusti, Pica, Cundy, Wenger, ...

They fit well the expected large-$N$ behavior: \( C = C_\infty + c_2/N^2 \), leading to \( C_\infty = 0.022(2) \), and \( c_2 \approx 0.06 \), corresponding to \( \chi^ {1/4}_\infty = 170(3) \text{MeV} \) using \( \sqrt{\sigma} = 440 \text{MeV} \), in substantial agreement with the large-$N$ WV formulae.
The $O(\theta^4)$ term of $f(\theta) \equiv (F(\theta) - F(0))/\sigma^2 = \frac{1}{2} C \theta^2 (1 + b_2 \theta^2 + \ldots)$

Large-$N$ scaling arguments predict $b_2 = O(N^{-2})$

Results for $N^2 b_2$ using various methods, $b_2 = -\chi_4/(12\chi)$ and $\chi_4 = \frac{1}{N} \left[ \langle Q^4 \rangle - 3\langle Q^2 \rangle^2 \right]_{\theta=0}$. They are consistent with $b_2 \approx \bar{b}_2/N^2$ with $\bar{b}_2 \approx -0.2$. (Del Debbio, Panagopoulos, V., D’Elia, Giusti, Petrarca, Taglienti)

$b_2$ is nonzero, $b_2 = -0.024(5)$ for $N = 3$, showing that there are deviations from a Gaussian distribution of $Q$.

$b_2$ turns out to be quite small. Deviations from a simple Gaussian behavior are already small at $N = 3$. For $N \geq 3$ $F(\theta) - F(0) \approx \frac{1}{2} \chi \theta^2$ provides a good approximation.
\( \theta \) dependence of the spectrum

The string tension, \( \sigma(\theta) = \sigma (1 + s_2 \theta^2 + ...) \), and the lowest glueball state, \( M(\theta) = M (1 + g_2 \theta^2 + ...) \), where \( M \) is the \( 0^{++} \) glueball mass at \( \theta = 0 \). At \( \theta \neq 0 \), the lightest glueball state becomes a mixed state of \( 0^{++} \) and \( 0^{-+} \) glueballs.

The coefficients can be computed from appropriate correlators at \( \theta = 0 \).

The large-\( N \) scaling arguments, which indicate that \( \bar{\theta} \equiv \theta/N \) is the scaling parameter in the large-\( N \) limit, imply that the coefficients of the \( \theta \) expansion are suppressed, i.e. \( s_2 \) and \( g_2 \) are \( O(N^{-2}) \).

Thus, the lowest spin-zero glueball state becomes a mixed state of \( 0^{++} \) and \( 0^{-+} \) glueballs, but its mass does not change.

This scenario is supported by lattice results for \( N = 3, 4, 6 \). Some estimates: \( s_2 = -0.08(1), g_2 = -0.06(2) \) for \( N = 3 \), decreasing with increasing \( N \) (Del Debbio, Manca, Panagopoulos, Skouroupathis, V.).
**θ dependence at finite temperature**

1st order transition from confined to unconfined phases for $N \geq 3$.

For $T \gg T_c$, $F(\theta) - F(0) \sim (1 - \cos \theta)T^4 \exp[-8\pi^2/g^2(T)]$, where $8\pi/g^2(T) \sim (11/3)N \ln T$, from the one-loop instanton contribution.

Lattice results for $\chi$ across the first order transition: the ratio $R(T) \equiv \chi(T)/\chi(T = 0)$ vs the reduced temperature $t \equiv T/T_c - 1$. $\chi$ and $b_2$ vary little up to $T \lesssim T_c$. They change across the transition, where $\chi$ shows a significant decrease.

At $T \gg T_c$ we expect $\chi \sim T^4 \exp[-8\pi^2/g^2(T)]$ from instantons.
Lattice results for $N = 3, 4, 6, 8$ (from Lucini, Teper, Wenger, Del Debbio, Panagopoulos, V) suggest the following large-$N$ scenario:

(●) the topological properties and their related quantities remain substantially unchanged in the low-$T$ confined phase.

(●) Across the first-order transition there is a sharp change of regime

(●) In the high-$T$ phase $\chi$ is largely suppressed. Such suppression becomes larger and larger with increasing $N$, suggesting that $\chi$ vanishes above $T_c$ in the large-$N$ limit.

At large $N$ the topological properties in the high-$T$ phase are essentially determined by instantons, from very high $T$ down to $T_c$; the exponential suppression of instantons, as $e^{-N}$, induces the rapid decrease of the topological activity observed in the large-$N$ limit (as originally proposed by Kharzeev, Pisarski, Tytgat).
**2D $CP^{N-1}$ models** as a theoretical laboratory

$$\mathcal{L} = \frac{N}{2g} D_{\mu} z D_{\mu} z, \quad D_{\mu} = \partial_{\mu} + i A_{\mu}, \quad A_{\mu} = i \bar{z} \partial_{\mu} z, \quad \bar{z} z = 1$$

where $z$ is a complex $N$-component scalar. They share several features with QCD: asymptotic freedom, gauge invariance, and topological structures (instantons, $\theta$ vacua).

Unlike 4D $SU(N)$ gauge theories, **systematic $1/N$ expansion**, keeping $g$ fixed, around the large-$N$ saddle-point solution.

**$\theta$ dependence:**

$$\mathcal{L}_\theta = \frac{N}{2g} D_{\mu} z D_{\mu} z - i \theta q(x), \quad q(x) = \frac{1}{2\pi} \epsilon_{\mu\nu} \partial_{\mu} A_{\nu}$$

$$F(\theta) = -\frac{1}{V} \ln \int [dA] \exp(- \int d^2 x \mathcal{L}_\theta)$$
\[ f(\theta) \equiv \xi^2[F(\theta) - F(0)], \]  
\[ \xi \]  
is a length scale defined at \( \theta = 0 \), from the second moment of  
\[ G_P(x - y) = \langle \text{Tr } P(x)P(0) \rangle \]  
with  
\[ P_{ij}(x) \equiv \bar{z}_i(x)z_j(x) \]  

\[ f(\theta) = \frac{1}{2} C \theta^2 \left( 1 + \sum_{n=1} b_{2n} \theta^{2n} \right) , \quad C \equiv \chi \xi^2, \quad \chi = \int d^2 x \langle q(0)q(x) \rangle. \]

Large-\( N \) scaling shows that the relevant variable is \( \bar{\theta} \equiv \theta/N \). Thus,

\[ f(\theta) = N \bar{f}(\bar{\theta} \equiv \theta/N), \quad \bar{f}(\bar{\theta}) = \frac{1}{2} \bar{C} \bar{\theta}^2 (1 + \sum_{n=1} \bar{b}_{2n} \bar{\theta}^{2n}), \]

where \( \bar{C} \equiv NC \) and \( \bar{b}_{2n} = N^{2n} b_{2n} = O(N^0) \).

This large-\( N \) scaling behavior is confirmed by \( 1/N \) calculations:

\[ f(\theta) = \frac{1}{4\pi N} \theta^2 + O(1/N^2) \]  
for \( |\theta| < \pi \),  
\[ C \equiv \chi \xi^2 = \frac{1}{2\pi N}, \]

\[ b_2 = -\frac{27}{5N^2} + O(1/N^3), \quad b_4 = -\frac{1830}{7N^4} + O(1/N^5). \]

Analogous results can be obtained for the spectrum.
Conclusions:

(•) Large-$N$ scaling arguments applied to $\theta$ dependence of 4D $SU(N)$ gauge theories,

$$f(\theta) \equiv [F(\theta) - F(0)]/\sigma^2 = \frac{1}{2}C\theta^2(1 + b_2\theta^2 + b_4\theta^4 + ...) = N^2\bar{f}(\theta/N)$$

$$C \equiv \chi/\sigma^2 = C_\infty + c_2/N^2 + ..., \quad b_2j = \bar{b}_2j/N^{2j} + ..., \quad \bar{b}_2j = \bar{b}_2j/N^{2j} + ...,$$

are fully supported by lattice results.

(•) Quantitative agreement with the Witten-Veneziano relation

$$\chi = \partial F(\theta)/\partial \theta^2|_{\theta=0} = \frac{f_\pi^2}{4N_f} \left(m_{\eta'}^2 + m_\eta^2 - 2m_K^2 \right),$$

arising from the large-$N$ solution of the $U(1)_A$ problem.