Θ dependence of 4D SU(N) gauge theories at finite temperature

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ABSTRACT: The dependence of 4D SU(N) gauge theories on the topological θ term is investigated at finite temperature, and in particular in the large-N limit. General arguments and numerical analyses exploiting the lattice formulation show that it drastically changes across the deconfinement transition. The low-T phase is characterized by a large-N scaling with θ/N as relevant variable, while in the high-T phase the scaling variable is just θ and the free energy is essentially determined by the instanton-gas approximation.

in collaboration with C. Bonati, M. D'Elia, H. Panagopoulos,

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

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

$q(x) = \frac{g^2}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}(x)F^a_{\rho\sigma}(x)$ is the topological charge density.

The topological θ term violates parity and time reversal

$|\theta| \lesssim 10^{-9}$ from experimental bounds on the neutron electric dipole moment: $|d_n| < 3\times 10^{-26}$ e cm, and $d_n \sim \theta e m_\pi^2/m_n^3 \approx 10^{-16}\theta\, e\,\mathrm{cm}$.

Nevertheless θ dependence remains an interesting issue,

for example, $U(1)_A$ problem $\rightarrow$ the axial $U(1)_A$ symmetry is not realized in the QCD spectrum, neither explicitly nor as a Goldstone mechanism ($m_{\eta'} > \sqrt{3}m_\pi$), being violated at quantum level

θ **dependence** vanishes in perturbation theory.

In the semiclassical picture, contributions from classical instanton solutions with nontrivial topology, $\int d^4x\, q[A_I(x)] = Q$, give rise to tunneling between n-vacua, leading to θ vacua: $|\theta\rangle = \sum_n e^{in\theta}|n\rangle$

The U(1)$_A$ charge is not conserved due to the chiral anomaly $\partial_\mu j_5^\mu(x) = i2N_f q(x)$.

A robust numerical evidence of a nontrivial θ dependence from MC simulations of the lattice formulation of the theory.

At finite T: this issue is related to the expected softening of the U(1)$_A$ breaking, to understand the main features of its T dependence, effective U(1)$_A$ symmetry restoration, T-dep of η' mass, nature of the hadron-to-quarkgluon transition, spectrum of the excitations, etc

possible evidences from heavy-ion collisions, e.g. claims of a softening of the η' mass from Au+Au collisions at RHIC (Csorgo *etal*, PRL 1010)

θ dependence of the ground-state and free energy

$T = 0$ ground-state energy:

$$E(\theta) = -\frac{1}{V_4} \ln \int [dA] \exp \left(- \int d^4x \mathcal{L}_\theta \right)$$

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

The free energy at finite temperature (Gross, Pisarski, Yaffe, RMP 1981)

$$F(\theta, T) = -\frac{1}{\mathcal{V}_4} \ln \mathrm{Tr} e^{-H/T} = -\frac{1}{\mathcal{V}_4} \ln \int [dA] \exp \left(- \int_0^{1/T} dt \int d^3x \, \mathcal{L}_\theta \right),$$

$$\mathcal{V}_4 \equiv T/V_3, \qquad A_\mu(1/T, \mathbf{x}) = A_\mu(0, \mathbf{x}), \qquad E(\theta) = F(\theta, 0)$$

In the pure gauge theory θ is a dimensionless RG invariant parameter, i.e. it does not renormalize in appropriate RG schemes, such as the $\overline{\mathrm{MS}}$ scheme

The ground-state/free energy can be parametrized as

$$\mathcal{F}(\theta,T) \equiv F(\theta,T) - F(0,T) = \frac{1}{2}\chi(T)\theta^2 s(\theta,T)$$

$\chi(T) = \int d^4x \langle q(x)q(0)\rangle_{\theta=0} = \langle Q^2\rangle_{\theta=0}/\mathcal{V}_4$ is the topological susceptibility, $s(\theta,T)$ is a dimensionless even function of θ such that $s(0,T)=1$.

Analyticity at $\theta = 0$ (CP is not broken at $\theta=0$, Vafa, Witten, PRL 1984) $\longrightarrow$

$$s(\theta,T) = 1 + b_2(T)\theta^2 + b_4(T)\theta^4 + \cdots\ ,$$ (V, Panagopoulos, PhysRep 2009)

b_i are dimensionless RG invariant quantities,

related to the zero-momentum n-point correlation functions of $q(x)$, e.g. $b_2 = -\chi_4/(12\chi)$ and $\chi_4 = \int d^4x_1 d^4x_2 d^4x_3 \langle q(0)q(x_1)q(x_2)q(x_3)\rangle_c|_{\theta=0}$, and the **cumulants** of $P(Q)$.

If $b_{2n}=0$ then the distribution is Gaussian $P(Q) = \frac{1}{\sqrt{2\pi\langle Q^2\rangle}}\exp\left(-\frac{Q^2}{2\langle Q^2\rangle}\right)$

Within the large-N framework ($N \to \infty$, $g^2 N$ fixed) the $\mathrm{U}(1)_A$ problem is explained by a θ dependence at the leading $1/N$ order

WV relations: $\chi = \frac{f_s^2 m_s^2}{4N_f}$ or $\frac{4N_f}{f_\pi^2}\chi = m_{\eta'}^2 + m_\eta^2 - 2m_K^2$ (Witten, Veneziano, 1979)

Large-N scaling to $\mathcal{L}_\theta = \frac{1}{4} F_{\mu\nu}^a(x) F_{\mu\nu}^a(x) - i\theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x)$
$\longrightarrow$ the relevant scaling variable is $\bar{\theta} \equiv \theta/N$

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

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

A multibranched $F(\theta)$, $F(\theta) - F(0) = \mathcal{A}\, \mathrm{Min}_k\, (\theta + 2\pi k)^2 + O\,(1/N)$ (Witten, AP 1980, PRL 1998), avoids the apparent incompatibility with periodicity in θ.

Semiclassically θ dependence arises from instantons.

The one-instanton contribution $e^{-8\pi^2/g^2}e^{i\theta} = \left(e^{-8\pi^2/(g^2N)}e^{i\theta/N}\right)^N$ suggests an exponentially small θ dep. **This conclusion is incorrect**: the instanton gas approximation fails due to infrared divergences.

At finite temperature, T **provides the infrared cutoff** to the instanton-size distribution, $n_I(\rho) \sim e^{-S(A_I)} \sim e^{-[8\pi^2/g^2+2N(\pi\rho T)^2]}$.

(Gross,Pisarski,Yaffe, RMP 1981)

Dilute instanton-gas (DIG) approximation at finite T summing over n_+ instantons and n_- antiinstantons:

$$\begin{aligned} Z_\theta &= \mathrm{Tr}\, e^{-H_\theta/T} \approx \sum \frac{1}{n_+!n_-!}(\mathcal{V}_4 D)^{n_++n_-} e^{-\frac{8\pi^2(n_++n_-)}{g^2}+i\theta(n_+-n_-)} \\ &= \exp\left[\cos\theta \times 2\mathcal{V}_4 D \times e^{-8\pi^2/g^2}\right] \end{aligned}$$

therefore $\mathcal{F}(\theta,T) \equiv F(\theta,T) - F(0,T) \approx \chi(T)\,(1-\cos\theta)$

At high T ... dilute instanton-gas (DIG) approximation

At one loop $\partial F/\partial\theta = \sin\theta \int_0^\infty d\rho\, n_{_I}(\rho) \sim \sin\theta \times T^4 e^{-8\pi^2/g^2(T)}$

$$\mathcal{F}(\theta,T) \approx \chi(T)\,(1-\cos\theta)\,, \qquad \chi(T) \approx T^4 \exp[-8\pi^2/g^2(T)] \sim T^{-\frac{11}{3}N+4},$$

using $8\pi^2/g^2(T) \approx (11/3)N\ln(T/\Lambda) + O(\ln\ln T/\ln^2 T)$

DIG is a good approximation when the overlap between instantons becomes negligible, thus at large T where $\chi(T)$ is suppressed

The high-T θ dependence qualitatively differs from that at $T=0$:

(•) analytic and periodic θ dependence

(•) The large-N scaling is not realized by the DIG approximation: the relevant variable for the instanton gas is θ, and **not** θ/N

(•) $\chi(T)$ gets exponentially suppressed in the large-N regime, suggesting a rapid decrease of the topological activity with increasing N at high T

• The low-T and high-T phases are separated by a **1$^{\rm st}$-order deconfinement transition**, at $T_c/\sqrt{\sigma} \approx 0.545(2) + 0.46(2)/N^2$ (Lucini, etal, 2004,2012) getting stronger with increasing N, $L_h \sim N^2$

• for $T \ll T_c \to$ large-N scaling with θ/N **as scaling variable** $\to$ $\chi/\sigma^2 \approx C_\infty + c/N^2$ and $b_k \approx \bar{b}_k/N^k$.

Does it extend up to T_c^-?

• for $T \gg T_c \to$ analytic θ dependence by DIG approximation: $\mathcal{F} \approx \chi(T)(1 - \cos\theta)$ with $\chi(T) \sim T^{-\frac{11}{3}N+4}$.

Does it extend down to T_c^+?

Working hypothesis: The change between the low-T and high-T θ dependence occurs around the deconfinement transition.

Some hints also from models like ADS-CFT, holographic models, etc... (Witten, PRL 1998; Parnashev, Zhitnisky PRD 1998; Unsal PRD 2012, etc)

Quantitative studies of θ dependence by MC simulations of the Wilson lattice formulation

$$Z = \int [dU] \exp(-S_L), \qquad S_L = -\frac{2a^4}{g_0^2} \sum \mathrm{ReTr}\,[U_\mu(x) U_\nu(x+a\hat{\mu}) U_\mu^\dagger(x+a\hat{\nu}) U_\nu^\dagger(x)]$$

The complex nature of the θ term prohibits MC simulations at $\theta \neq 0$.

Expansion around $\theta = 0$: $\qquad F(\theta) - F(0)) = \frac{1}{2}\chi\theta^2(1 + b_2\theta^2 + b_4\theta^4 + ...)$

χ and b_{2n} from correlation functions $\langle q(x_1) q(x_2) ... q(x_{2n})\rangle$ at $\theta = 0$,

$$b_2 = -\frac{\chi_4}{12\chi}, \qquad \chi_4 = \frac{1}{V}\left[\langle Q^4\rangle - 3\langle Q^2\rangle^2\right]_{\theta=0}, \qquad Q = \sum_x q(x)$$

$$b_4 = \frac{\chi_6}{360\chi}, \qquad \chi_6 = \frac{1}{V}\left[\langle Q^6\rangle - 15\langle Q^2\rangle\langle Q^4\rangle + 30\langle Q^2\rangle^3\right]_{\theta=0}$$

In the continuum limit, $b_{2k,L} \approx b_{2k} + a^2\sigma^2$ for $a \to 0$

$b_{2n} \longrightarrow$ deviations from a Gaussian $P(Q) = \frac{1}{\sqrt{2\pi\langle Q^2\rangle}} \exp\left(-\frac{Q^2}{2\langle Q^2\rangle}\right)$

Various methods to compute Q, based on smoothing, off-equilibrium, fermionic index, GW Dirac operators, ...

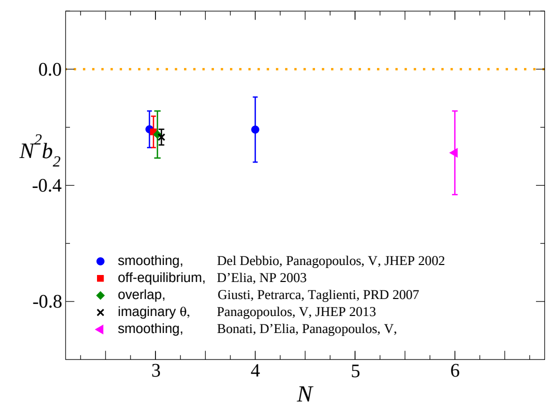
θ dependence at $T = 0$

- $\chi \equiv \partial^2 F(\theta)/\partial\theta^2|_{\theta=0} \neq 0$ for SU(3): $\chi/\sigma^2 = 0.028(2)$ by various methods

- **Nonzero large-N limit**: $\chi/\sigma^2 = 0.022(2)$, investigated by MC simulations for $N > 3$ (by Cundy, Del Debbio, Lucini, Panagopoulos, Teper, V., Wenger, ... They support the expected large-N behavior: $\chi/\sigma^2 = C_\infty + c_2/N^2$

- **Nonzero higher-order terms** of the expansion around $\theta = 0$,

$F(\theta) - F(0) = \frac{1}{2}\chi\theta^2(1 + b_2\theta^2 + b_4\theta^4 + ...)$,
SU(3) estimates: $b_2 = -0.026(3)$ and $|b_4| \lesssim 0.001$
(using various methods to determine Q)



- **Vanishing large-N limit** of $b_k = O(N^{-k})$,
results consistent with $b_2 \approx \bar{b}_2/N^2$, $\bar{b}_2 \approx -0.2$,
see the plot of $N^2 b_2$ vs N

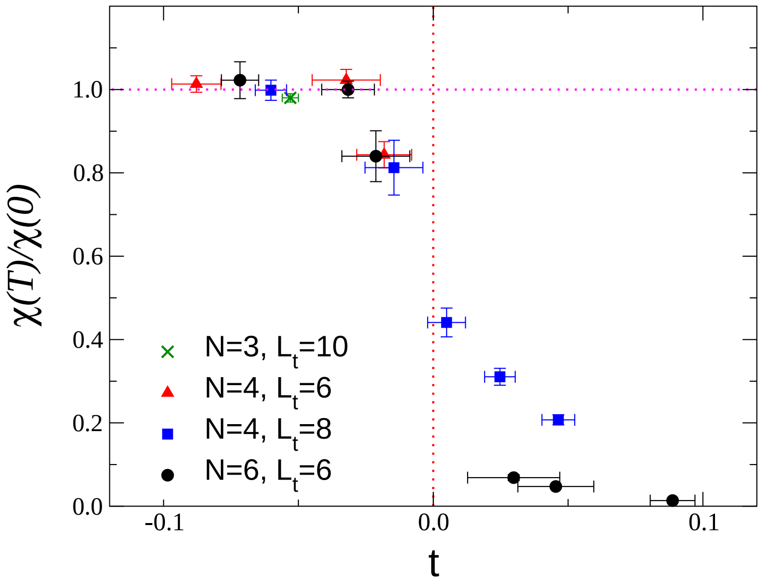
Deviations from a simple Gaussian behavior are already small at $N = 3$.

b_k requires large statistics, due to the cancellation of volume factors

• χ **at finite** T

Several MC results (Alles, Bonati, Del Debbio, D'Elia, Di Giacomo, Lucini, Panagopoulos, Teper, V., Wenger, ...)

$\chi(T)/\chi(T=0)$ vs $t \equiv T/T_c - 1$ across the transition $\longrightarrow$



• χ remains substantially unchanged in the low-T confined phase.

This also suggests $T_c(\theta) \approx T_c + c\,\theta^2/N^2$ (D'Elia, Negro, PRL 2012)

• A sharp change across the first-order transition, likely discontinuous

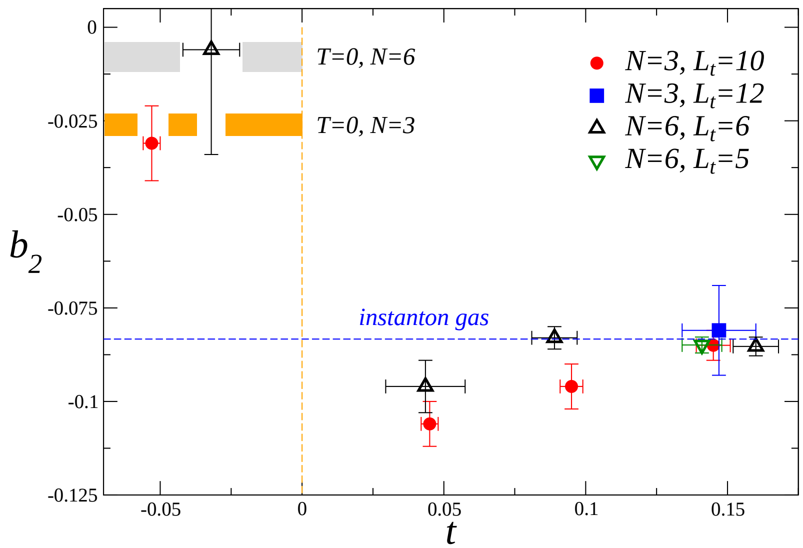
• In the high-T phase χ shows a clear suppression, which becomes stronger with increasing N, in qualitative agreement with one-loop DIG $\chi(T) \sim T^{-\frac{11}{3}N+4}$ for $T \gg T_c$, but larger T are necessary for a quantitative check of the one-loop DIG approximation of $\chi(T)$

• Higher-order terms of $F(\theta,T) = \frac{1}{2}\chi\theta^2(1 + b_2\theta^2 + b_4\theta^4 + \cdots)$ provide a more significant probe of DIG regimes, avoiding the problem of the logarithmic corrections of the prefactor

High-statistics MC for $N = 3, 6$ and $L_t = 5, 6, 10, 12$ (smoothing techniques for Q), to check large-N scaling and continuum limit.

(Bonati, D'Elia, Panagopoulos, V, PRL 2013)

b_{2k} are compared with $T = 0$ results and DIG approx $\longrightarrow$



• Sharp change across the deconfinement transition, likely discontinuous

• For $T > T_c$, **rapid approach to DIG θ dependence**, with deviations visible only for $t \approx 0.05$. The approach appears faster with increasing N.

• $b_4 = 0.0024(4)$ for $N = 6$ and $t = 0.09$ to be compared with $b_4 = 1/360$.

Deviations from dilute instanton gas at $t \equiv (T - T_c)/T_c \lesssim 0.1$

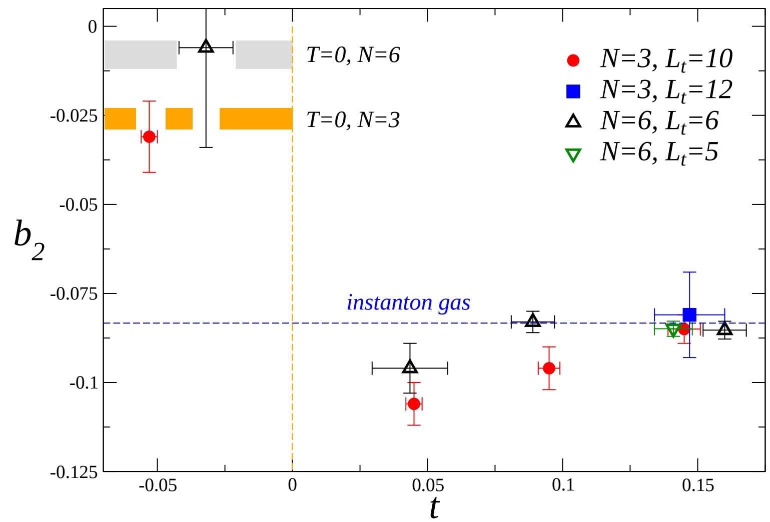
The approach to the DIG regime can be parametrized by a virial-like expansion: the asymptotic formula is corrected by a term proportional to the square of the instanton density

Since $\chi(T) \sim \rho_{\rm inst}$,

$\mathcal{F}(\theta, T) \approx \chi(1 - \cos\theta) + \chi^2 \kappa(\theta) + O(\chi^3)$

$\kappa(\theta) = \sum_{k=2} c_{2k} \sin(\theta/2)^{2k}$

Thus, $b_2 = -\frac{1}{12} + \frac{1}{8} c_4 \chi + O(\chi^2)$.



The behavior $\chi \sim T^{-11N/3+4}$ implies a rapid approach to the asymptotic DIG value, which becomes faster with increasing N.

The hard-core approximation of instanton interactions give a negative correction, i.e. $c_4 < 0$, explaining the approach from below to the DIG value $b_2 = -1/12$.

Summary of the θ dependence in 4D SU(N) gauge theories

$$\mathcal{F}(\theta,T) \equiv F(\theta,T) - F(0,T) = \frac{1}{2}\chi(T)\theta^2 \left(1 + b_2(T)\theta^2 + b_4(T)\theta^4 + \cdots\right)$$

• **Low-T phase** characterized by a **large-N scaling** with θ/N as relevant variable: $\chi/\sigma^2 \approx C_\infty + c/N^2$ and $b_k \approx \bar{b}_k/N^k$

• **Sharp change across the deconfinement transition**, likely discontinuous, which becomes sharper with increasing N.

• **High-T phase**: large-N scaling is lost, the topological activity is largely reduced. **The dilute instanton-gas regime sets in just above T_c**, giving an analytic dependence $F(\theta) - F(0) \approx \chi(T)(1 - \cos\theta)$.

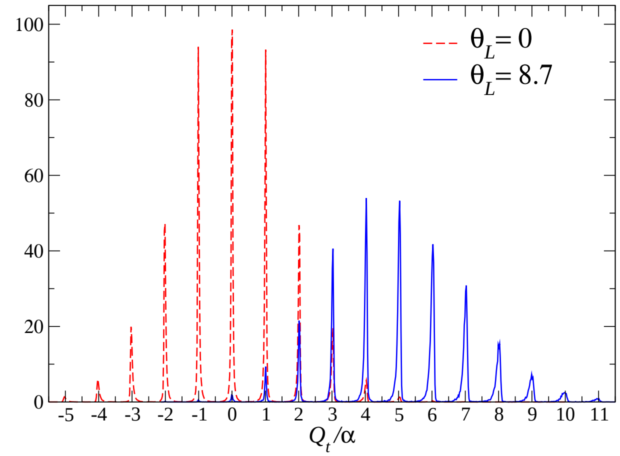
• MC simulations nicely support the above scenario.

• Analog results expected in full QCD, which would imply suppressed $\mathrm{U}(1)_A$ breaking in the quark-gluon plasma. Around T_c, this may affect the nature of the chiral transition, because a suppressed $U(1)_A$ breaking would lead to the $[U(2)_L \otimes U(2)_R]/U(2)_V$ universality class, different from $O(4)/O(3)$.

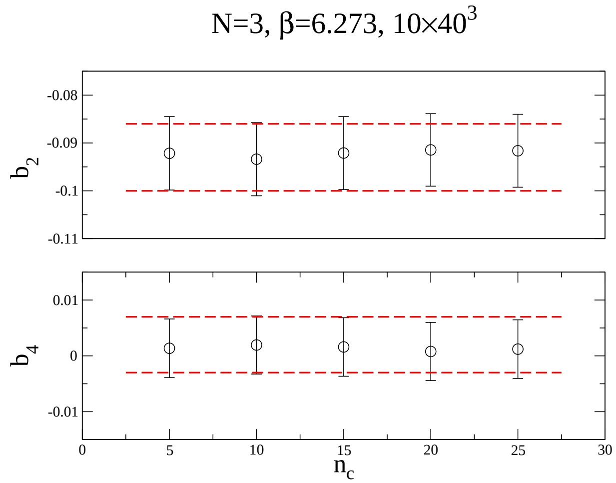
Further slides ...

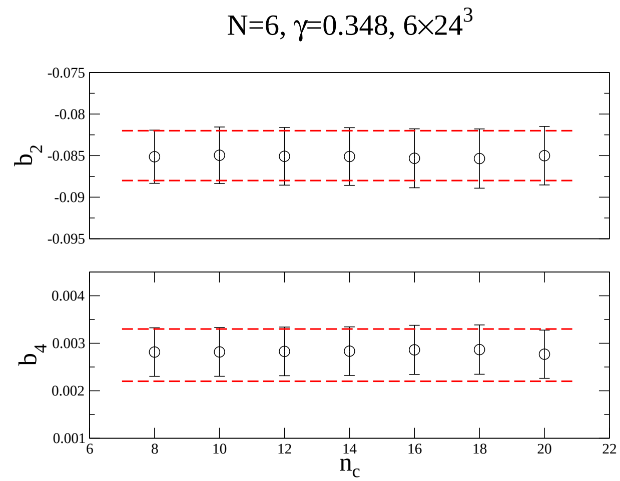
Some results from the smoothing method.

Distribution of Q, for $N=3$, $\beta=6.2$ at $\theta=0$ and $\theta_i \approx 1.5$



Stability of the lattice computation of b_2 in the high-T phase, for $N=3$ and $N=6$





Semiclassically θ dependence arises from instantons

Nontrivial θ dependence from the expansion of the functional integral in the sector with $Q = n$ about the minimum action with $Q = n$.

$$Z = \mathrm{Tr}\, e^{-H/T} = \int \mathcal{D}A e^{-S(A)+i\theta Q(A)}$$

$$= \sum_n e^{i\theta n} \int \mathcal{D}A \delta(Q-n) e^{-S(A)} \approx \sum_n e^{i\theta n} \int du\, e^{-S(A_I(u))} \mathrm{Det}[Q(A_I(u))]$$

Instantons: classical finite-energy solutions $A_I(u)$ which minimize the action within each topological sector, tunneling among n-vacua

$$A_I^\mu = 2\eta^{\mu\nu,a}\tau^a \frac{x_\nu}{x^2+\rho^2}, \qquad S(A_I) = 8\pi^2/g^2$$

The one-instanton contribution $e^{-8\pi^2/g^2} e^{i\theta} = \left(e^{-8\pi^2/(g^2 N)} e^{i\theta/N}\right)^N$ appears exponentially suppressed in the large-N limit, suggesting that the θ dependence is exponentially small in N.

This conclusion is incorrect, the instanton gas approximation fails due to infrared divergences.

Dilute instanton-gas (DIG) approximation at finite T

At finite T, due to electric screening, only fields with integer Q can contribute to the functional integral: **periodic instantons** in $\beta = 1/T$

(Gross, Pisarski, Yaffe, RMP 1981)

$$A_I^\mu = \Pi \bar{\eta}^{\mu\nu,a}(\tau^a/2i)\partial_\nu \Pi^{-1}, \qquad \Pi(t,\mathbf{x}) = 1 + \frac{(\pi\rho^2 T/r)\sinh(2\pi T r)}{\cos(2\pi T r) - \cosh(2\pi T t)}$$

At finite temperature, T plays the role of infrared cutoff,

$n_I(\rho) \sim e^{-S(A_I)} \sim e^{-[8\pi^2/g^2 + 2N(\pi\rho T)^2]}$

DIG approximation summing over n_+ instantons and n_- antiinstantons:

$$\begin{aligned} Z_\theta &= \mathrm{Tr}\, e^{-H_\theta/T} \approx \sum \frac{1}{n_+! n_-!} (\mathcal{V}_4 D)^{n_+ + n_-} e^{-\frac{8\pi^2(n_+ + n_-)}{g^2} + i\theta(n_+ - n_-)} \\ &= \exp\left[\cos\theta \times 2\mathcal{V}_4 D \times e^{-8\pi^2/g^2}\right] \end{aligned}$$

therefore $\mathcal{F}(\theta, T) \equiv F(\theta, T) - F(0, T) \approx \chi(T)\,(1 - \cos\theta)$