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

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We report a study of the dependence of 4D SU(N) gauge theories on the topological θ term at finite temperature, and in particular in the large-N limit. We show that the θ dependence drastically changes across the deconfinement transition. The low-temperature phase is characterized by a large-N scaling with θ/N as relevant variable, while in the high-temperature phase the free energy is essentially determined by the dilute instanton-gas approximation, with a simple θ dependence of the free-energy density $F(\theta,T)-F(0,T)\sim 1-\cos\theta$.

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4D SU(N) gauge theories have a nontrivial dependence on the topological θ term which can be added to the standard Euclidean Lagrangian, i.e.

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

where $q(x)$ is the topological charge density. The θ term is phenomenologically important, because it breaks both parity and time reversal. Its experimental upper bound within the strong-interaction theory is very small, $|\theta| < 10^{-9}$ [1]. Nevertheless, the θ dependence is an interesting physical issue, relevant to hadron phenomenology, an example being the so-called U(1)$_A$ problem. Indeed, the nontrivial θ dependence provides an explanation to the fact that the U(1)$_A$ symmetry of the classical theory is not realized in the hadron spectrum [2, 3, 4]. The θ dependence at finite temperature (T) is related to the issue of the effective restoration of the U(1)$_A$ symmetry in strong interactions at finite T, at high T and around the chiral transition, which may be also relevant to the nature of the transition itself [5, 6].

We report a study [7] of the θ dependence of 4D SU(N) gauge theories at finite T, in particular across the deconfining temperature T_c. The finite-T behavior is specified by the free-energy density

$$F(\theta,T) = -\frac{1}{\mathscr{V}}\ln\int[dA]\exp\left(-\int_0^{1/T}dt\int d^3x\mathscr{L}_\theta\right), \tag{2}$$

where $\mathscr{V} = V/T$ is the Euclidean space-time volume, and the gluon field satisfies $A_\mu(1/T,\mathbf{x}) = A_\mu(0,\mathbf{x})$. The θ dependence can be parameterized as

$$\mathscr{F}(\theta,T) \equiv F(\theta,T) - F(0,T) = \frac{1}{2}\chi(T)\theta^2 s(\theta,T), \tag{3}$$

where $\chi(T)$ is the topological susceptibility at $\theta = 0$,

$$\chi = \int d^4x \langle q(x)q(0)\rangle_{\theta=0} = \frac{\langle Q^2\rangle_{\theta=0}}{\mathscr{V}}, \tag{4}$$

and $s(\theta,T)$ is a dimensionless even function of θ such that $s(0,T) = 1$. Assuming analyticity at $\theta = 0$, $s(\theta,T)$ can be expanded as

$$s(\theta,T) = 1 + b_2(T)\theta^2 + b_4(T)\theta^4 + \cdots, \tag{5}$$

where only even powers of θ appear.

At $T = 0$, where the free energy coincides with the ground-state energy, large-N scaling arguments [2, 8, 9] applied to the Lagrangian (1) indicate that the relevant scaling variable is $\bar\theta \equiv \theta/N$, i.e. $\mathscr{F}(\theta) \approx N^2\mathscr{G}(\bar\theta)$ as $N \to \infty$. Comparing with Eq. (3), this implies the large-N behavior

$$\chi/\sigma^2 = C_\infty + O(N^{-2}), \quad b_{2j} = \bar b_{2j}/N^{2j} + O(N^{-2j-2}), \tag{6}$$

where σ is the string tension, C_∞ and $\bar b_{2j}$ are large-N constants. A nonzero value of C_∞ is essential to provide an explanation to the U(1)$_A$ problem in the large-N limit [3, 4].

The large-N scaling (6) is not realized by the dilute instanton gas (DIG) approximation. Indeed, at $T = 0$, instanton calculations fail due to the fact that large instantons are not suppressed.

On the other hand, the temperature acts as an infrared regulator, so that the instanton-gas partition function is expected to provide an effective approximation of finite-T SU(N) gauge theories at high T [10], high enough to make the overlap between instantons negligible. The corresponding θ dependence is [10, 11]

$$\mathscr{F}(\theta,T) \equiv F(\theta,T) - F(0,T) \approx \chi(T)\,(1-\cos\theta)\,, \tag{7}$$

$$\chi(T) \approx T^4 \exp[-8\pi^2/g^2(T)] \sim T^{-\frac{11}{3}N+4}, \tag{8}$$

using $8\pi^2/g^2(T) \approx (11/3)N\ln(T/\Lambda) + O(\ln\ln T/\ln^2 T)$. Therefore, the high-$T$ θ dependence substantially differs from that at $T=0$: the relevant variable for the instanton gas is just θ, and not θ/N. The DIG approximation also shows that $\chi(T)$, and therefore the instanton density, gets exponentially suppressed in the large-N regime, thus suggesting a rapid decrease of the topological activity with increasing N at high T. Since the instanton density gets rapidly suppressed in the large-N limit, making the probability of instanton overlap negligible, the range of validity of the DIG approximation is expected to rapidly extend toward smaller and smaller temperatures with increasing N. An interesting question is how and when the DIG regime sets in.

In 4D SU(N) gauge theories the low-T and high-T phases are separated by a first-order deconfinement transition which becomes stronger with increasing N [12], with T_c converging to a finite large-N limit: [13] $T_c/\sqrt{\sigma} = 0.545(2) + O(N^{-2})$. This suggests that the change from the low-T large-N scaling θ dependence to the high-T DIG θ dependence occurs around the deconfinement transition. See, e.g., Refs. [14, 15, 16, 17] for further discussions of this scenario.

Due to the nonperturbative nature of the physics of θ dependence, quantitative assessments of this issue have largely focused on the lattice formulation of the SU(N) gauge theory, using Monte Carlo (MC) simulations. However, the complex character of the θ term in the Euclidean QCD Lagrangian prohibits a direct MC simulation at $\theta \neq 0$. Information on the θ dependence of physically relevant quantities, such as the ground state energy and the spectrum, can be obtained by computing the coefficients of the corresponding expansion around $\theta = 0$, which can be determined by computing appropriate zero-momentum correlation functions of the topological charge density at $\theta = 0$ [18, 19]. For example,

$$\chi_l = \frac{\langle Q^2\rangle}{\mathscr{V}}, \qquad b_2 = -\frac{\langle Q^4\rangle - 3\langle Q^2\rangle^2}{12\langle Q^2\rangle}, \qquad b_4 = \frac{\langle Q^6\rangle - 15\langle Q^2\rangle\langle Q^4\rangle + 30\langle Q^2\rangle^3}{360\langle Q^2\rangle}, \tag{9}$$

where Q is topological charge, χ_l is the the lattice topological susceptibility ($\chi_l \approx a^4\chi$; a is the lattice spacing). The coefficients b_i in Eq. (5) are dimensionless and renormalization-group invariant, therefore they approach their continuum limit with $O(a^2)$ corrections.

We mention that issues related to θ dependence, particularly in the large-N limit, can also be addressed by other approaches, such as AdS/CFT correspondence applied to nonsupersymmetric and nonconformal theories, see e.g. Refs. [8, 17, 20, 21], and semiclassical approximation of compactified gauge theories [22, 23].

The large-N scaling of the θ dependence is fully supported by numerical computations exploiting the nonperturbative Wilson lattice formulation of the 4D SU(N) gauge theory at $T=0$, see, e.g., the results reported in Table 1 for $N=3,4,6$ (see also Refs. [9, 25] for recent reviews). A large-N extrapolation of these data, using $a + b/N^2$ and b/N^{2j} for χ/σ^2 and b_{2j} respectively, leads

N	χ/σ^2	b_2	b_4
3	0.028(2) [9]	$-0.026(3)$ [24]	0.000(1) [24]
4	0.0257(10) [18]	$-0.013(7)$ [18]	
6	0.0236(10) [18]	$-0.008(4)$ [7]	0.001(3) [7]

Table 1: Summary of known $T = 0$ results for the ratio χ/σ^2 (where σ is the $\theta = 0$ string tension) and the first few coefficients b_{2j} for $N = 3,4,6$. More complete reviews of results can be found in Refs. [9, 25]; in particular other results for b_2 at $N = 3$ are reported in Refs.[18, 26, 27].

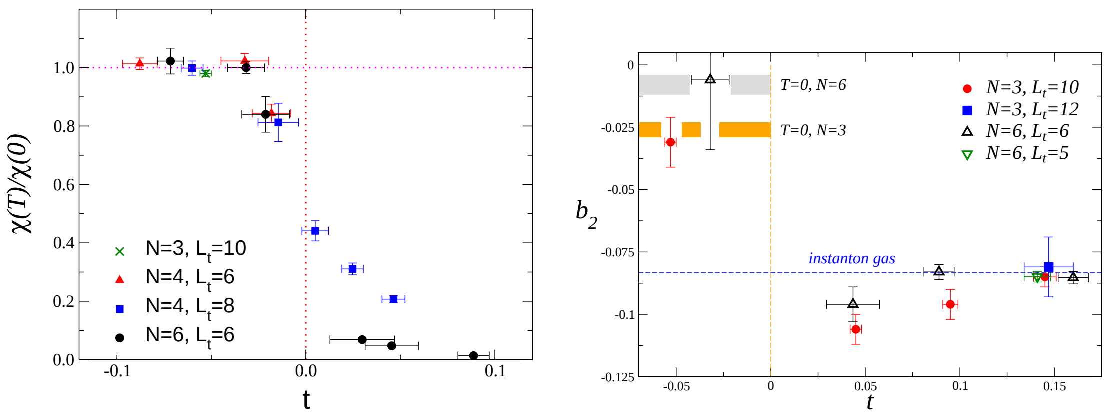

Figure 1: The ratio $\chi(T)/\chi(0)$ between the topological susceptibility at T and zero temperature (left) and the coefficient b_2 of the free-energy expansion around $\theta = 0$ (right), versus the reduced temperature $t \equiv T/T_c - 1$, around the deconfinement transition corresponding to $t = 0$. We show data for various values of N and lattice sizes $L_t \times L_s^3$ with $L_s/L_t \geq 4$, where L_t, L_s are respectively the number of sites along the *time* and *space* directions. The shadowed regions in the right figure indicate the $T = 0$ estimates of b_2 for $N = 3$ and $N = 6$. The data for $N = 4$ of the left figure are taken from Ref. [15].

to the estimates

$$C_\infty = \lim_{N\to\infty} \chi/\sigma^2 = 0.022(2), \qquad \bar{b}_2 = \lim_{N\to\infty} N^2 b_2 = -0.23(2). \tag{10}$$

This large-N scenario is expected to remain stable against sufficiently low temperatures.

The finite-T lattice investigations of the large-N behavior of $\chi(T)$ [28, 15, 29, 30] indicate a nonvanishing large-N limit for $T < T_c$, remaining substantially unchanged in the low-T phase, from $T = 0$ up to T_c. Across T_c a sharp change is observed, and $\chi(T)$ appears largely suppressed in the high-T phase $T > T_c$, in qualitative agreement with a high-T scenario based on the DIG approximation. Some MC data are shown in Fig. 1 (left panel).

A more stringent check of the actual scenario realized in 4D SU(N) gauge theories is provided by the higher-order terms of the expansion (5). Indeed, the expansion coefficients b_{2j} are expected to scale like N^{-2j} if the free energy is a function of θ/N and to be N-independent in the DIG approximation, or, more generally, if the relevant large-N scaling variable is just θ. In particular, the simple θ dependence of Eq. (7) may be observed at much smaller T above T_c with respect to the asymptotic one-loop behavior (8) of $\chi(T)$ which is subject to logarithmic corrections.

We computed the first few coefficients of the expansion (5) around T_c, for $N = 3$ and $N = 6$ to check the N dependence, using the lattice Wilson formulation of SU(N) gauge theories, and a smearing technique to determine the topological charge. They require high-statistics simulations due to the cancellation of volume factors in their definitions (9). For details see Ref. [7]. Fig. 1 (right panel) shows the data for b_2. The MC results clearly show a change of regime in the θ dependence, from a low-T phase where the susceptibility and the coefficients of the θ expansion vary very little, to a high-T phase where the coefficients b_{2j} approach the instanton-gas predictions. In the high-T phase they are definitely not consistent with the large-N scaling in Eq. (6), which would imply a factor of four in b_2, in going from $N = 3$ to $N = 6$. On the other hand, in the low-T phase b_2 does not significantly differ from the $T = 0$ value. This is consistent with the behaviour of the topological susceptibility, see the left panel of Fig. 1. Although our MC results in the high-T phase are obtained for relatively small reduced temperatures $t \equiv T/T_c - 1$, i.e. $t < 0.2$, the data for b_2 show a clear and rapid approach to the value $b_2 = -1/12$ of the instanton gas model for both $N = 3$ and $N = 6$, with significant deviations visible only for $t \lesssim 0.1$. The high-T values of b_2 substantially differ from those of the low-T phase, and in particular from those at $T = 0$ reported in Table 1. Also the estimates of b_4 are consistent with the small value $b_4 = 1/360$. The sharp behavior of the θ dependence at the phase transition suggests that T_c is actually a function of θ/N at finite θ, as put forward in Ref. [31].

A virial-like expansion can account for the deviations for b_2, visible at $t \lesssim 0.1$, by correcting the asymptotic formula by a term proportional to the square of the instanton density. For example, we may write

$$\mathscr{F}(\theta,T) \approx \chi(1-\cos\theta) + \chi^2\kappa(\theta) + O(\chi^3), \tag{11}$$

using the fact that $\chi(T)$ is proportional to the instanton density, and $\kappa(\theta)$ can be parametrized as $\kappa(\theta) = \sum_{k=2} c_{2k}\sin(\theta/2)^{2k}$. The above formula gives $b_2 \approx -1/12 + \frac{1}{8}c_4\chi/T_c^4$. This predicts a rapid approach to the asymptotic value of the DIG approximation, since χ gets rapidly suppressed in the high-T phase, as suggested by Eq. (8) and confirmed by the MC results. Moreover, a hard-core approximation of the instanton interactions [11] gives rise to a negative correction, i.e. $c_4 < 0$, explaining the approach from below to the perfect instanton-gas value $b_2 = -1/12$.

This numerical analysis provides strong evidence that the θ dependence of 4D SU(N) gauge theory experiences a drastic change across the deconfinement transition, from a low-T phase characterized by a large-N scaling with θ/N as relevant variable, to a high-T phase where this scaling is lost and the free energy is essentially determined by the DIG approximation, which implies an analytic and periodic θ dependence. The corresponding crossover around the transition becomes sharper with increasing N, suggesting that the DIG regime sets in just above T_c at large N.

In full QCD the θ dependence is closely related to the effective breaking of the U(1)$_A$ symmetry, through the axial anomaly which is proportional to the topological charge density, i.e. $\partial_\mu J_5^\mu(x) \propto \frac{1}{N}q(x)$ in the chiral limit. Its effects around the chiral transition may be relevant to the nature of the transition itself. In the light-quark regime the nature of the finite-temperature transition is essentially related to the restoring of the chiral symmetry, and the corresponding symmetry breaking pattern [5]. In the relevant case of two light flavors, this is $\mathrm{SU}(2)_L \otimes \mathrm{SU}(2)_R \to \mathrm{SU}(2)_V$, thus equivalent to O(4)$\to$O(3). On the other hand, if the effects of the axial anomaly are effectively suppressed at the transition, the relevant symmetry breaking is $\mathrm{U}(2)_L \otimes \mathrm{U}(2)_R \to \mathrm{U}(2)_V$. This implies that, in the case of a continuous chiral transition (note however that the transition may be also first order independently of the symmetry breaking), the critical behavior belongs to different 3D universality classes in the two cases [32, 33].

Analogously to pure gauge theories, semiclassical instanton calculations predict a substantial suppression of the instanton density at large temperatures, $T \gg T_c$ say, where the DIG model is expected to provide a reliable approximation [10]. For example, in QCD with two light flavors of mass m, the topological susceptibility χ is expected to asymptotically decrease as $\chi \sim m^2 T^{-\kappa}$, with $\kappa = \frac{11}{3}N - \frac{16}{3}$. Although χ vanishes in the massless limit, the Dirac zero modes associated with the instantons induce a residual contribution to the $\mathrm{U}(1)_A$ symmetry breaking, giving rise to a difference between the susceptibilities of the so-called π and δ channels at high T, [34, 35] which behaves as $\chi_\pi - \chi_\delta \sim T^{-\kappa}$ in the chiral limit. Therefore, the DIG approximation suggests that the $\mathrm{U}(1)_A$ symmetry is not exactly recovered at finite T, although its breaking gets largely suppressed with increasing the temperature.

The breaking of the $\mathrm{U}(1)_A$ symmetry at finite temperature has been much investigated, even numerically by MC simulations of lattice QCD, see e.g. Refs. [34, 35, 36, 37, 38, 39, 40] and references therein. These studies agree with a substantial suppression of the $\mathrm{U}(1)_A$ anomaly effects at large temperature, as predicted by the DIG model. This scenario is strenghtened by our numerical investigation of the pure $\mathrm{SU}(N)$ gauge theories. However, the issue about the significance of this suppression around the chiral transition is still debated.

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