θ dependence in the large N limit

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Outline

1. Introduction to θ dependence
2. Results in the literature
3. Numerical methods
4. Our results

The θ term

The Euclidean Yang-Mills Lagrangian with the topological term is

$$\mathcal{L}_\theta^E = \frac{1}{4} F^{a\,\mu\nu}(x) F^a_{\mu\nu}(x) - i\theta q(x)$$

$$q(x) \equiv \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F^{a\,\mu\nu} F^{a\,\rho\sigma}$$

and the main features of $q(x)$ are

$$q(x) = \partial_\mu K^\mu(x), \qquad Q = \int q(x) \mathrm{d}x \in \mathbb{Z} \ .$$

- θ is an RG invariant parameter
- Sign problem for $\theta \neq 0$, $\theta \in \mathbb{R}$.

How does the free (or ground state) energy depends on θ?
General properties:

- $F(-\theta, T) = F(\theta, T)$
- $F(\theta, T) \geq F(0, T)$

General parametrization of the θ dependence

Assuming analyticity at $\theta = 0$ and using $F(T, -\theta) = F(T, \theta)$ we have

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

The coefficients can be written using only expectation values computed at $\theta = 0$ as ($\langle \cdots \rangle_0 = \langle \cdots \rangle_{\theta=0}$)

$$\chi = \frac{1}{V_4}\langle Q^2\rangle_0 \qquad b_2 = -\frac{\langle Q^4\rangle_0 - 3\langle Q^2\rangle_0^2}{12\langle Q^2\rangle_0}$$

$$b_4 = \frac{\langle Q^6\rangle_0 - 15\langle Q^2\rangle_0\langle Q^4\rangle_0 + 30\langle Q^2\rangle_0^3}{360\langle Q^2\rangle_0}$$

Coefficients b_{2n} parametrize the deviations of the distribution of topological charge from a Gaussian in the theory at $\theta = 0$.

Large N scaling

$$F^a_{\mu\nu}F^{a\,\mu\nu} \text{ and } \epsilon_{\mu\nu\rho\sigma}F^{a\,\mu\nu}F^{a\,\rho\sigma} \text{ scale as } N^2$$

To have a nontrivial θ dependence in the large N limit we have to keep $\bar{\theta} \equiv \theta/N$ fixed, in such a way that θg^2 does not scale with N

Assuming the large N limit not to be singular, the large N scaling form of the free energy is thus (Witten 1980)

$$F(\theta, T) - F(0, T) = N^2 \bar{F}(\bar{\theta}, T)$$

where $\bar{F}$ has the (asymptotic) expansion:

$$\bar{F}(\bar{\theta}, T) = \frac{1}{2}\bar{\chi}\bar{\theta}^2\left[1 + \bar{b}_2\bar{\theta}^2 + \bar{b}_4\bar{\theta}^4 + \cdots\right] .$$

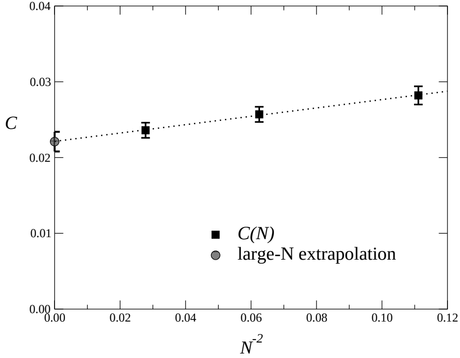
By matching the powers of θ we obtain

$$\chi = \bar{\chi} + O(1/N^2)$$
$$b_{2n} = \bar{b}_{2n}/N^{2n} + O(1/N^{2n+2})$$

Large N scaling of χ

Del Debbio, Panagopoulos, Vicari 0204125

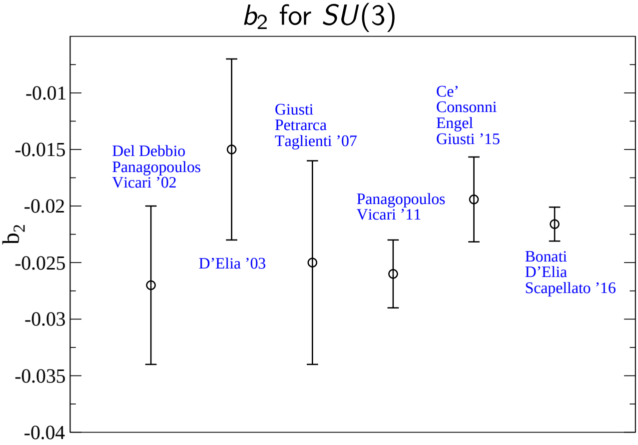
$C = \chi/\sigma^2, \ T = 0$



(see also Lucini, Teper, 0103027)

The main source of error is the value of the string tension. To improve these results it is sufficient to have a more precise scale setting.

b_2 estimates



For $N > 3$: $b_2|_{SU(4)} = -0.013(7)$ and $b_2|_{SU(6)} = -0.01(2)$
from Del Debbio, Panagopoulos, Vicari 0204125.

b_{2n}s are dimensionless: errors are (almost) independent of scale settings.

Why is it difficult to evaluate b_{2n}? (1)

General problems for all topological observables

- Topology is well defined only in the continuum limit.
  Several possible way out, we used cooling as smoother (see e.g. Panagopoulos, Vicari 0803.1593, Bonati, D'Elia 1401.2441 for comparison of different procedures).
  Asymptotic freedom and topology ensures the correctness of virtually all procedures as the continuum limit is approached.

- Large autocorrelation times.
  In theories without fermions this problem is less important but it gets worse and worse as the number of colors increases.
  We had to use very large statistics (for $SU(6)$ around 6×10^7 updates, 1 update = 1 heatbath + 5 overrelaxation).

Why is it difficult to evaluate b_{2n}? (2)

Specific problem for b_{2n}: lack of self-averaging. Consider e.g.

$$b_2 = -\frac{\langle Q^4\rangle_0 - 3\langle Q^2\rangle_0^2}{12\langle Q^2\rangle_0}$$

In the thermodynamical limit the probability distribution of Q is dominated by Gaussian fluctuation of typical size $\delta Q \sim \sqrt{\chi V_4}$, the mean value of the numerator grows $\sim V_4$, while its error $\sim \chi^2 V_4^2$.
For b_4 and higher b_{2n}s the scaling is even worst.

Standard solution: do not study fluctuation observables "at zero external field", study instead the response to an external field (Milchev, Binder, Heermann 1986).

In this case "external field" = nonvanishing θ. To avoid the sign problem use $\theta = i\theta_I$, with $\theta_I \in \mathbb{R}$ (Vicari, Panagopoulos 1109.6815).

Details of the numerical procedure adopted

The adopted action was (S_W is the usual Wilson action)

$$S[U] = S_W[U] - \theta_L Q_L[U], \quad Q_L = \sum_x q_L(x)$$

$$q_L(x) = -\frac{1}{2^9\pi^2} \sum_{\mu\nu\rho\sigma=\pm1}^{\pm4} \tilde{\epsilon}_{\mu\nu\rho\sigma} \mathrm{Tr}\left(\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)\right) \ .$$

θ_L gets a finite renormalization ($\theta_I = Z\theta_L$) and Z, χ, b_{2n} have been evaluated by fitting together the first four cumulants of Q:

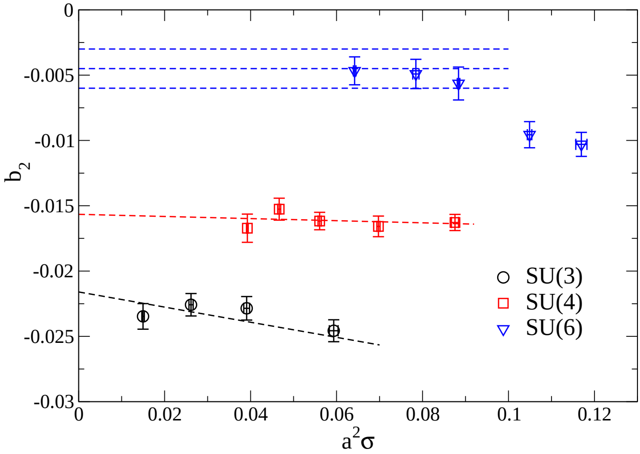
$$\frac{\langle Q\rangle}{\mathcal{V}} = \chi Z\theta_L(1 - 2b_2Z^2\theta_L^2 + 3b_4Z^4\theta_L^4 + \dots),$$

$$\frac{\langle Q^2\rangle_c}{\mathcal{V}} = \chi(1 - 6b_2Z^2\theta_L^2 + 15b_4Z^4\theta_L^4 + \dots),$$

$$\frac{\langle Q^3\rangle_c}{\mathcal{V}} = \chi(-12b_2Z\theta_L + 60b_4Z^3\theta_L^3 + \dots),$$

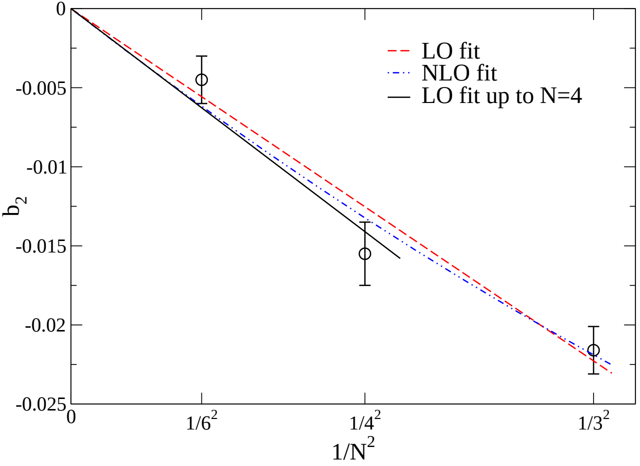
$$\frac{\langle Q^4\rangle_c}{\mathcal{V}} = \chi(-12b_2 + 180b_4Z^2\theta_L^2 + \dots).$$

Results for b_2 in $SU(4)$ and $SU(6)$



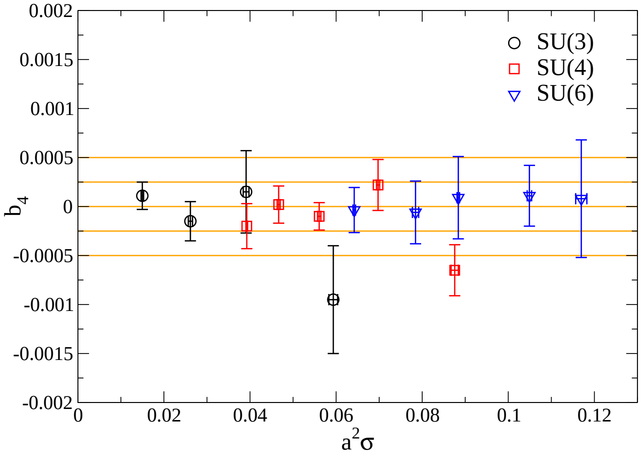
$$b_2|_{SU(4)} = -0.0155(20)$$
$$b_2|_{SU(6)} = -0.0045(15)$$
$(b_2|_{SU(3)} = -0.0216(15)$ (C. Bonati, M. D'Elia, A. Scapellato 1512.01544))

Large N scaling of b_2



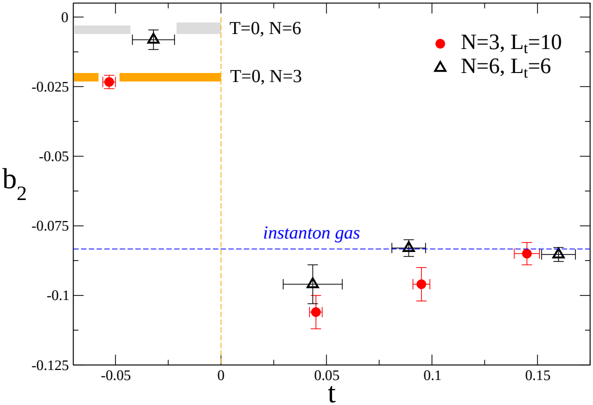
With a fit $b_2 = \bar{b}_2/N^2$ on $N \geq 4$ one gets $\bar{b}_2 = -0.23(3)$, NLO corrections are compatible with zero and using $b_2 = c_1/N^{2c_2}$ one gets $c_2 = 1.0(2)$.

b_4 bounds



$b_4 \lesssim 5 \times 10^{-4}$ is a conservative bound for all N values.

Why checking large N scaling?



C. Bonati, M. D'Elia, H. Panagopoulos, E. Vicari 1301.7640, (C. Bonati, M. D'Elia, A. Scapellato 1512.01544, Bonati, D'Elia, Rossi, Vicari 1607.06360)

Since sometimes it fails! For $T > T_c$ b_2 is almost independent on N.

Conclusion

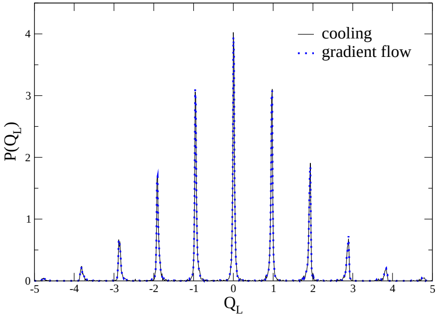
- The b_{2n} coefficients characterize the θ dependence of the free (or ground state) energy and they are challenging to estimate.
- We presented the first numerical determination of b_2 for $SU(4)$ and $SU(6)$ performed with enough accuracy to verify the large N scaling
- We presented stringent bound for b_4 in $SU(4)$ and $SU(6)$
- The method adopted can be useful also in finite temperature simulations, especially for $T < T_c$, and we applied it to refine our previous study of the change of θ dependence at T_c.

Thank you for your attention!

Backup slides with something more

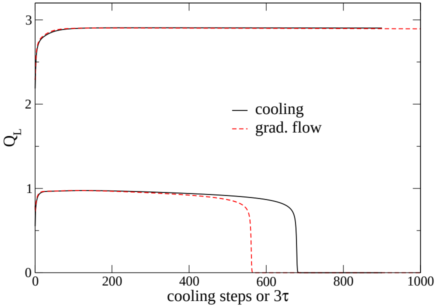
Comparison between smoothing algorithms

Bonati, D'Elia 1401.2441



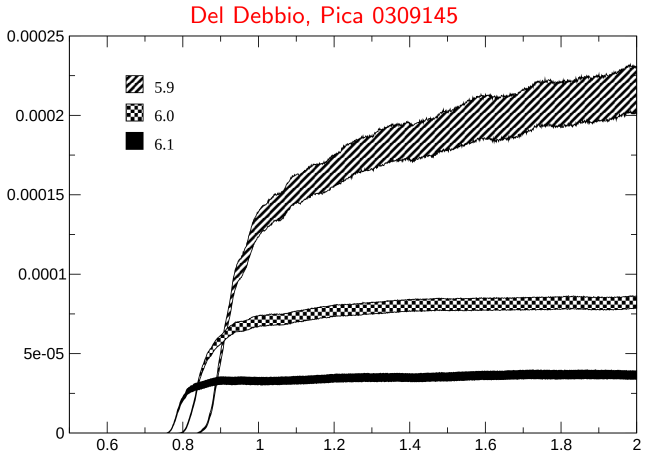
Topological charge distribution obtained by cooling or gradient flow in $SU(3)$ at $\beta = 6.2$.

Bonati, D'Elia, Rossi, Vicari 1607.06360



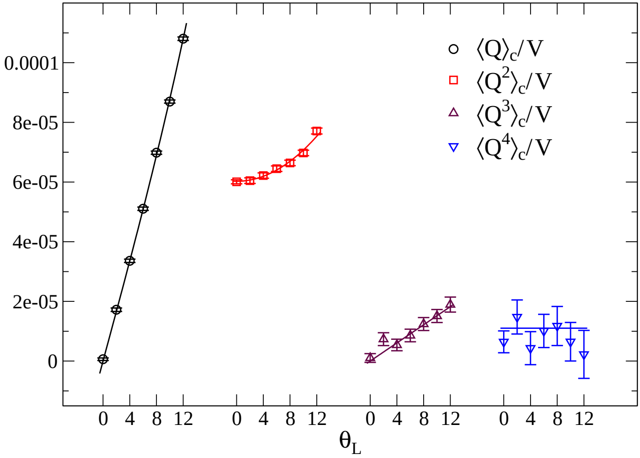
Evolution of Q_L under cooling and gradient flow in $SU(6)$ at $\beta = 24.056$.

Overlap ambiguities



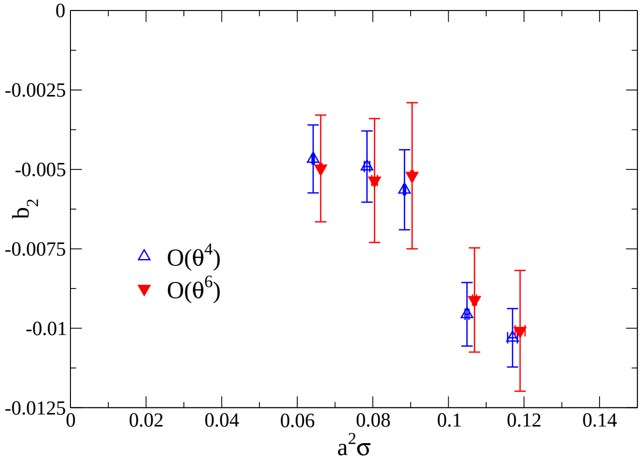
Cooling-like picture displaying the values of the top. susceptibility as a function of the mass used in the overlap Dirac operator in $SU(3)$.

Example of the global fit procedure



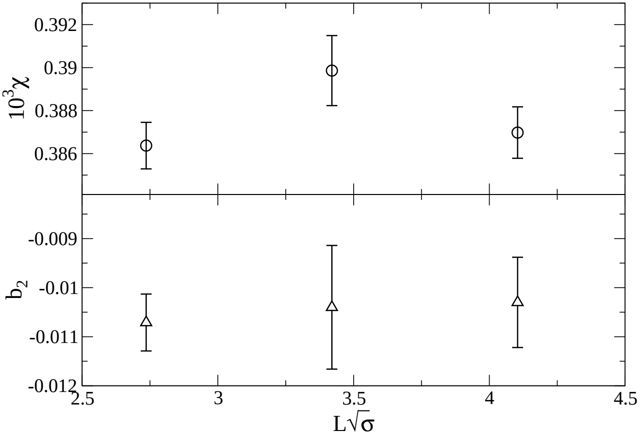
Common fit to the first four cumulants of the topological charge for $SU(4)$ at coupling $\beta = 11.008$.

Truncation systematics



Test for systematics using two different truncation orders for $SU(6)$.

Finite volume effects



Test for finite size effects in $SU(6)$ at coupling $\beta = 24.500$.

Dilute Instanton Gas Approximation

In general one has (e.g. Coleman "The uses of instantons")

weak coupling approximation ⇒ semiclassical approximation

Slightly broader perspective:

possibility that a system can be described by means of weakly interacting classical configurations even if the "elementary" coupling is not small

For weakly interacting instantons we have (DIGA, Gross, Pisarski, Yaffe 1981)

$$Z_\theta = \mathrm{Tr} e^{-H_\theta/T} \approx \sum \frac{1}{n_+!n_-!}(V_4 D)^{n_+ + n_-} e^{-S_0(n_+ + n_-) + i\theta(n_+ - n_-)}$$
$$= \exp\left[2 V_4 D e^{-S_0}\cos\theta\right]$$

where $1/D$ is a typical $4-$volume. Thus

$$F(\theta, T) - F(0, T) \approx \chi(T)(1 - \cos\theta)$$