The topological properties of QCD at high temperature: problems and perspectives

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35th International Symposium on Lattice Field Theory
Granada (Spain), 19-24 June 2017

What we would like to do

First principle computation of the θ dependence of the free energy density

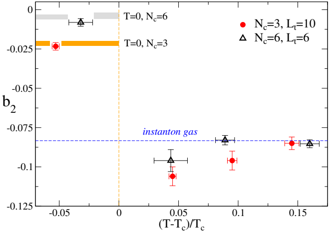
$$f(\theta, T) = f(\theta = 0, T) + \frac{1}{2}\chi(T)\theta^2\Big(1 + b_2(T)\theta^2 + \cdots\Big)$$

In terms of observables at $\theta = 0$ we have

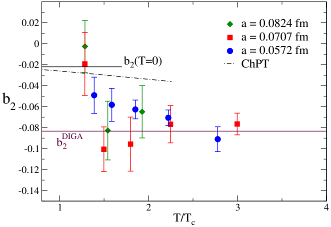
$$\chi(T) = \langle Q^2\rangle_0 / V_4; \qquad b_2(T) = \Big(\langle Q^4\rangle_0 - 3\langle Q^2\rangle_0^2\Big) \Big/ \Big(12\langle Q^2\rangle_0\Big)$$

DIGA: $f(\theta, T) - f(\theta = 0, T) = \chi(T)\big(1 - \cos\theta\big)$ (thus $b_2 = -1/12$)

DIGA + perturbation theory: $\chi(T) \propto m_q^{N_f}\, T^{4 - \frac{11}{4}N_c - \frac{1}{3}N_f}$



Bonati, D'Elia, Panagopoulos, Vicari 1301.7640
(and 1512.01544 and 1607.06360)



Bonati et al. 1512.06746

The problems

The study of the topological properties of QCD at high temperature is a challenging task mainly because of the following problems:

Freezing of Q the autocorrelation time of the topological charge Q grows very quickly with $1/a$ ($\sim$ exponentially)

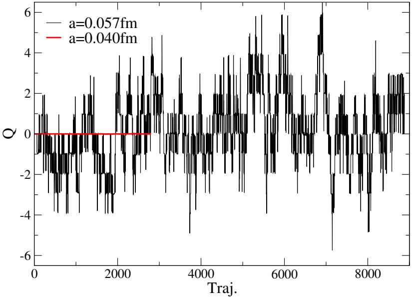
Finite volume in the high temperature limit $\chi(T) \to 0$ and it is very difficult to sample the $Q \neq 0$ sectors ($\delta Q \sim \sqrt{\chi V_4}$)

These are serious difficulties even in YM theory, but in that case we have better algorithms and much larger statistics Berkowitz, Buchoff, Rinaldi 1505.07455; Kitano, Yamada 1506.00370; Borsanyi et al. 1508.06917

A peculiar feature of the theory with light fermions is the very slow convergence to the continuum of χ (at least with non chiral fermions)

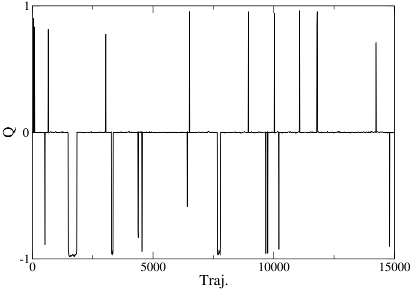
Moreover $\chi_{QCD} \ll \chi_{YM}$, thus worsening the finite volume problem.

The problems



$T = 0$ case: several Q values for "large" a values, freezed in a single sector for smaller a

$T \simeq 310\mathrm{MeV}$ with $a \simeq 0.040\mathrm{fm}$ on a 16×64^3 lattice: the $Q = 0$ sector is strongly favoured, some spurts at $Q = \pm 1$, some freezing (at $Q = -1$).



Wishlist

1. improve the convergence to the continuum
(larger lattice spacings can be used, reduce the need for solving the freezing problem)

2. improve the decorrelation of Q
(solve or at least alleviate the freezing problem, important also to ensure ergodicity in "non topological" simulations, possibility of performing brute force continuum limit)

3. cope with the $Q \neq 0$ suppression at large T
(enable topology to be studied directly at large T, avoiding the use of extrapolations)

Speeding up the continuum limit

- $T = 0$ solution: from χPT we know that the improved observable is $\chi = \chi_L \times (m_\pi^{\rm phys}/m_\pi^{\rm ts})^2$, where χ_L is the value actually measured in the simulation and $m_\pi^{\rm ts}$ is the taste singlet pion mass

  Bonati et al. 1512.06746; Borsanyi et al. 1606.07494

- $T > 0$ solution (1^{st} try): at fixed lattice spacing, use the dimensionless ratio $\chi(a, T)/\chi(a, T = 0)$ Bonati et al. 1512.06746
  This procedure seems to remove the $a-$dependence but in fact it shifts the problem to smaller lattice spacings.

  Petreczky, Schadler, Sharma 1606.03145; Borsanyi et al. 1606.07494

- $T > 0$ solution (2^{nd} try): eigenvalue reweighting Borsanyi et al. 1606.07494
  identify would-be zero modes of $\not{D}$ (would = without chiral violation) and force them to zero. What about the other modes? In particular, what about near-zero modes? (e.g. when $Q = 0$, $n_+ = 1$, $n_- = 1$)

Fighting the freezing

Several strategies are being studied, an (incomplete) list is

change b.c.
- open b.c. Lüscher, Schaefer 1105.4749
- "Moebius" b.c. Mages et al. 1512.06804

tempering
- simulated/parallel tempering Vicari 9209025, Hasenbusch 1706.04443

multi-can.
- plain multicanonical (*)
- metadynamics (*) Laio, Martinelli, Sanfilippo 1508.07270
- density of states (*)

fixed Q
- sub-volume methods Brower et al. 1403.2761 Bietenholz, Forcrand, Gerber 1509.06433,
- from Q dependence (*) Brower et al. 0302005, Aoki et al. 0707.0396
- "thermodynamical integration" of Z_Q/Z_0 (*) Frison et al. 1606.07175, Borsanyi et al. 1606.07494

Algorithms (*) also solve the "Q=0" problem at high temperature.

By now almost unexplored possibility: use more than a single method.

Metadynamics

Metadynamics has been introduced to efficiently sample the configuration space of models with several free energy minima and in which we have some understanding of the relevant degrees of freedom (i.e. no spin glass)

The philosophy of metadynamics is the following Laio, Parrinello 0208352

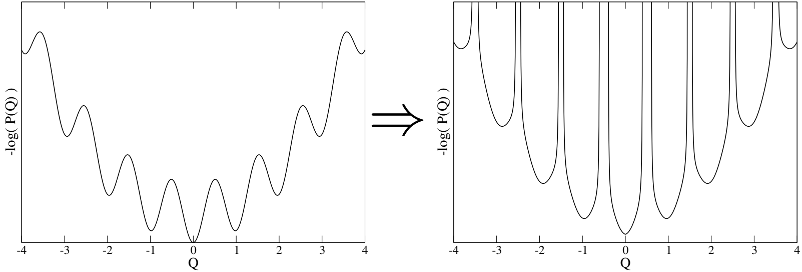
1. identify the "slow variable" ϕ (typically called "collective variable")
2. introduce in the Hamiltonian an external history-dependent potential for the slow variable $V(\phi, t)$ ($t =$ Monte Carlo time)
3. during the update modify $V(\phi, t)$ in such a way that the distribution of ϕ is constant in the interval of interest $[\phi_{\mathrm{min}}, \phi_{\mathrm{max}}]$
4. at the end reweight data with $\overline{V(\phi, t)}$, that is an estimator of the free energy at fixed ϕ

The method is closely related to the multicanonical method:
pro: the motion in configuration space is a biased random walk (faster)
con: no more a stationary process (in fact no more a Markov Chain)

Application to topology in QCD

The natural choice for the slow variable is the topological charge Q, however this presents some problems:

- geometric or fermionic definitions of Q cannot be used, since they do not generate biasing forces
- even if the Q defined after smoothing is not exactly integer, its distribution is very strongly peaked close to integer values



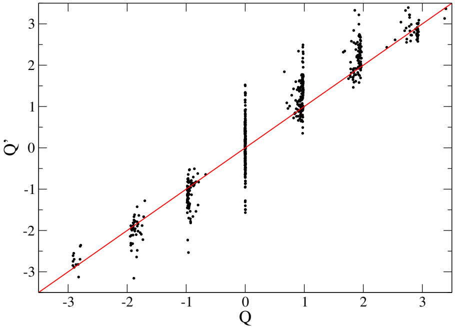
The intuitive idea of "mountain-passing" bias potential is not valid for Q

Application to topology in QCD

We need to find an "interpolating" observable Q' such that

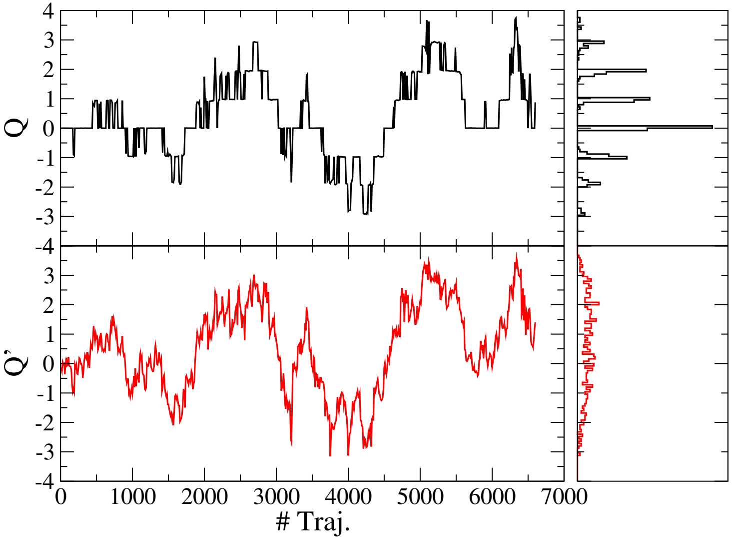
- it is smooth enough to be used as slow-variable in the bias potential
- it is correlated enough with the topological charge Q to propagate the effect of the bias to the topology

Simple guess: we can use as Q' the under-smoothed topological charge, i.e. the discretized $F\tilde{F}$ operator measured after few smoothing steps.



In this example ($T \simeq 310\,\mathrm{MeV}$, $a \simeq 0.040\,\mathrm{fm}$) Q is measured after 70 cooling steps and it is in the plateau region, Q' is measured after 20 stout smearing steps with $\alpha = 0.1$

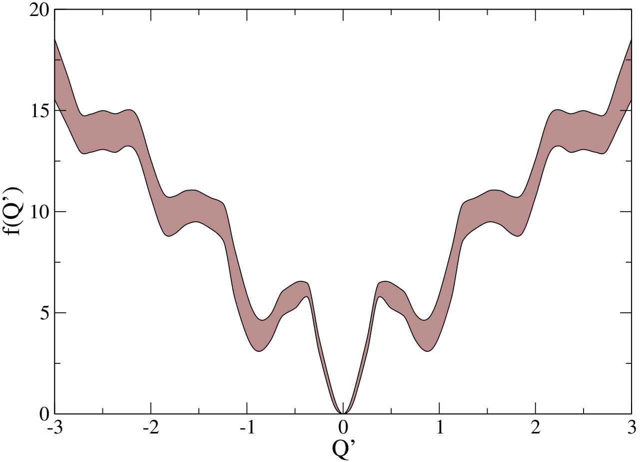
Application to topology in QCD



$T \simeq 310\text{MeV}$, $a \simeq 0.040\text{fm}$, 16×64^3 lattice, metapot. for $Q' \in [-3, 3]$

Application to topology in QCD

The free energy density at fixed Q'



$T \simeq 310\mathrm{MeV}$, $a \simeq 0.040\mathrm{fm}$, 16×64^3 lattice, metapot. for $Q' \in [-3, 3]$

Conclusion and perspectives

Different methods to quantitatively investigate the topological properties of QCD at high temperature are by now available.

The metadynamical approach has resulted to be quite effective in

- favouring tunneling between different topological sectors
- improving the sampling of the $Q \neq 0$ sectors at high temperature

The overhead introduced by metadynamics was at most a $\times 3$ factor in all the studied cases.

The possibility of using different methods now open the possibility of cross-checking the pysical results and gaining insight into the sistematics of the different approaches.

Thank you for your attention!