Simple check of the vacuum structure in full QCD lattice simulations

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Abstract. Given the increasing availability of lattice data for (unquenched) QCD with \( N_f = 2 \), it is worth while to check whether the generated vacuum significantly deviates from the quenched one. I discuss a specific attempt to do this on the basis of topological susceptibility data gained at various sea-quark masses, since for this observable detailed predictions are available. The upshot is that either discretization effects in dynamical simulations are still intolerably large or the vacuum structure in 2-flavour QCD substantially deviates from that in the theory with 3 (or 2+1) light quarks.

INTRODUCTION

In a historical perspective, the path towards phenomenological predictions of QCD by means of lattice techniques involves three steps: Pure Yang-Mills theory (where there is just glueball physics), quenched QCD (where the vacuum is the one in the SU(3) theory, but observables may involve so-called current-quarks) and full QCD (where the fermion determinant with the dynamical sea-quarks accounts for the quark loops in the vacuum).

Today, the lattice community makes the final push towards full QCD, despite the fact that state-of-the-art simulations are modestly announced as “partially quenched” which means that the sea- and current-quark masses in the (euclidean) generating functional

\[
Z[\bar{\eta}, \eta] = \int DA \ e^{-S_G} \prod_{N_f} \det(D + m_{\text{sea}}) \exp\left(\int \bar{\eta} \frac{1}{D + m_{\text{cur}}} \eta\right) \quad (1)
\]

are (in general) unequal and in most cases significantly heavier than the physical \( u \)- and \( d \)-quarks, so that phenomenological statements require a twofold extrapolation.

Since the finite sea-quark mass constitutes the key ingredient in this ultimate step (note that the determinant turns into a constant for \( m_{\text{sea}} \to \infty \), hence (1) reduces to the quenched generating functional in that limit), an obvious task is to check whether these “partially quenched” or “full” QCD simulations exhibit the change in the vacuum structure expected to occur if the fermions are “active” (i.e. if the back-reaction of the “dynamical” fermions on the gauge background is taken into account). The prime observable used to distinguish the respective vacua is the topological susceptibility

\[
\chi(m_{\text{sea}}) = \frac{\langle q^2 \rangle}{V}, \quad (2)
\]

with \( q \) the (global) topological charge, because detailed theoretical predictions show that \( \chi \) behaves rather different in the quenched (\( m_{\text{sea}} \to \infty \)) and chiral (\( m_{\text{sea}} \to 0 \)) limits,
respectively. Even though in the lattice-regulated theory (and with certain definitions of the topological charge operator) $q$ may be somewhat ambiguous on the level of a single configuration, the moment of the $q$-distribution which enters (2) can be measured with controlled error-bars, and as a purely gluonic object the resulting $\chi = \chi(m_{\text{sea}})$ encodes nothing but the vacuum structure of the theory.

Below, I give a quick survey of recent lattice determinations of $\chi$ at various sea-quark masses in $N_f = 2$ QCD, I discuss the available continuum knowledge of the functional form $\chi = \chi(m_{\text{sea}})$, and I present a non-standard lattice determination of the quenched topological susceptibility $\chi_{\infty}$ and the chiral condensate $\Sigma$ based on it. The outcome is that either certain observables in today’s phenomenological studies with light dynamical quarks suffer from large discretization effects or – the more speculative view – that the low-energy structure of QCD with $N_f = 2$ is substantially different from that with $N_f = 3$.

**LATTICE DATA**

I start with a quick survey of recent lattice data for the topological susceptibility in QCD with 2 dynamical flavours; the selection reflects nothing but my personal awareness.

**CP-PACS:** The CP-PACS collaboration has simulated full QCD on several grids at various $(\beta, \kappa)$-values, using an RG-improved gauge action and an $O(a)$-improved fermion action with mean-field values for the associate $c_{\text{SW}}$ coefficients. Below, I concentrate on the data generated on the $24^3 \times 48$ lattice at $\beta = 2.1$ with LW-cooling [1].

**UKQCD:** The UKQCD collaboration has simulated full QCD on a $16^3 \times 32$ grid at various $(\beta, \kappa)$-values, using the standard (Wilson) gauge action and an $O(a)$-improved fermion action with the non-perturbative values for the associate $c_{\text{SW}}$ coefficients [2].

**SESAM/TXL:** The SESAM/TXL collaboration has simulated full QCD on two grids ($16^3 \times 32$ and $24^3 \times 40$) at several $(\beta, \kappa)$-values, combining the unimproved (Wilson) gauge action with unimproved (Wilson) fermions (i.e. setting $c_{\text{SW}} = 0$) [3].

**Thin link staggered:** Trusting a continuum identity for the relationship between the 2- and the 4-flavour functional determinant, the staggered fermion action may be used to simulate QCD with $N_f = 2$. There are data by the Pisa group [4] and by A. Hasenfratz based on configurations by the MILC collaboration and the Columbia/BNL project [5].

Fig. 1 displays the data, along with continuum constraints to be discussed next.

**CONTINUUM KNOWLEDGE**

As mentioned in the introduction, the data for the topological susceptibility $\chi$ versus the sea-quark mass $m \equiv m_{\text{sea}}$ prove useful to test the vacuum structure, because continuum QCD provides us with detailed predictions: There are analytic upper bounds for $\chi(m)$ at both asymptotically small and large sea-quark masses and there is a “semi-analytic” formula for $\chi(m)$ valid at intermediary quark masses (where the bulk of the lattice data reside). The only caveat is that these bounds hold true in the continuum limit, but so far no continuum extrapolation for $\chi(m)$ in $N_f = 2$ QCD is available yet. Before stating the complications due to this, the continuum functional forms shall be discussed.
Asymptotically small sea-quark masses: For \( m \ll \Lambda_{\text{QCD}} \) and to leading order in the chiral expansion the axial WT-identity yields (see Refs. cited in [6] for details)

\[
\chi(m) = \frac{\sum m}{N_f} (1 + O(m)) = \frac{M_\pi^2 F_\pi^2}{2N_f} (1 + O(m)) \equiv \chi_0 (1 + O(m)),
\]

where, in the second equality, the Gell-Mann–Oakes–Renner relation has been assumed.

Asymptotically large sea-quark masses: For \( m \gg \Lambda_{\text{QCD}} \) the topological susceptibility gradually approaches its quenched counterpart (see Refs. cited in [6] for details)

\[
\chi(m) = \chi_\infty (1 + O(1/m)) = (200 \pm 5 \text{MeV})^4,
\]

Intermediate quark masses: For other quark masses (i.e. for \((M_\pi r_0)^2 \in [1.5, 15]\) or so, with the Sommer scale \( r_0 = 0.5 \text{ fm} \) throughout) neither one of the asymptotic predictions is applicable. Fortunately, there is the “reduced” interpolation formula

\[
\chi(m) = 1/(1/\chi_0 + 1/\chi_\infty)
\]

with \( \chi_0 \) defined in (3), which is, of course, not exact but represents an “educated guess”; it follows either from the chiral Lagrangian together with pure entropy considerations (which makes it very robust) [6] or from large-\( N_c \) arguments [7].
FIGURE 2. Topological susceptibility versus quark mass in $N_f = 2$ QCD with Wilson-type (left) or staggered (right) sea-quarks [1, 2, 3, 4, 5] together with naive fits of the susceptibility curve (5) to the data, neglecting possible discretization effects. The associate values for $\Sigma$ and $\chi_\infty$ are tabulated in Table 1.

NAIVE EVALUATION OF $\Sigma_2$ AND $\chi_\infty$

Disregarding possible lattice artefacts, one may fit the available data to the continuum curve (5) and extract $\Sigma$ and $\chi_\infty$ from the fit parameters [6]. It is worth emphasizing that this evaluation of $\Sigma$ is distinct from the usual fermionic determination which is via the trace of the Green’s function of the Dirac operator at various current-quark masses and extrapolating (after proper renormalization) to the physical (or chiral) point. Regardless how convincing this sounds, the results as tabulated in Table 1 look rather devastating: While our value for the quenched topological susceptibility $\chi_\infty \simeq (200 \pm 10 \text{MeV})^3$ nicely agrees with previous direct determinations in the SU(3)-theory, the suggested value for the (full) chiral condensate in the chiral limit $\Sigma \simeq (450 \pm 100 \text{MeV})^3$ dramatically exceeds (by more than a factor 2) the “phenomenological” value $\Sigma \simeq (288 \text{MeV})^3$ (which follows from the GOR-relation with $m_{u,d}(\overline{\text{MS}}, \mu = 2 \text{GeV}) \simeq 3.5 \text{MeV}$ [8]).

Looking back at Fig. 1, one may argue that this hardly comes as a surprise, since both the “Wilson-type” and the “staggered” data sets are much more likely to violate the linear upper bound in the deep chiral regime than the flat ceiling in the heavy-(sea)-quark limit. Besides, Fig. 1 tells us how important it is to compare the data to the right prediction: Knowing nothing but the chiral constraint (3), one might be tempted to say that the data are in nice agreement with the leading order chiral prediction. The outcome
TABLE 1. Naive determination of $\Sigma$ and $\chi_\infty$ from full QCD vacuum data with (5), using $r_0 = 0.5$ fm and the GOR-relation to convert to physical units.

|                  | CP-PACS | UKQCD   | SESAM * | PISA    | BOULDER |
|------------------|---------|---------|---------|---------|---------|
| $(F_\pi r_0)^2/4$ | 0.0417  | 0.0216  | 0.1600  | 0.1728  | 0.0441  |
| $F_\pi [\text{MeV}]$ † | 161.  | 116.  | 316.  | 32B.  | 166.  |
| $\Sigma^{1/3} [\text{MeV}]$ | 415. | 334. | 650. | 667. | 423. |
| $\chi_\infty r_0^4$ | 0.0616  | 0.0781  | 0.0587  | 0.0343  | 0.0748  |
| $\chi^{1/4}_\infty [\text{MeV}]$ | 197. | 209. | 194. | 170. | 206. |

* All data get equal weights, otherwise the best direct fit is almost flat (cf. Fig. 2).
† Using the convention in which $F_\pi \simeq 93$ MeV in nature; note that – except for the one in the UKQCD column – all entries are substantially larger than that value.

of our analysis shows that there is absolutely no point in comparing lattice data gained at $(M_\pi r_0)^2 \geq 1.5$ to the leading order chiral behaviour (3), because the “true” prediction (5) is substantially lower: If lattice data at $(M_\pi r_0)^2 = 2.5$ are found to be in “nice agreement” with the chiral prediction (3) based on the phenomenological value $\Sigma \simeq (288 \text{ MeV})^3$, then it means that they are $\sim 50\%$ in excess of what they should be.

The bottom line is that today’s full QCD simulations (with both Wilson-type and staggered sea-quarks) – if taken at face value – do show unquenching effects in their vacuum structure but, in general, far less than expected at their respective sea-quark masses. Unpleasant as it is, we are invited to think about the reasons for this finding.

TWO ALTERNATIVES

There are two main reasons why $\Sigma$ as determined via fitting full QCD topological susceptibility data to (5) could substantially exceed the standard phenomenological value $\Sigma \simeq (288 \text{ MeV})^3$ while the simultaneously determined $\chi_\infty$ takes a regular value.

**Large lattice artefacts:** The simple reason is that discretization effects could be large, since for the case of the topological susceptibility finite-volume effects are analytically shown to be well under control in most of today’s simulations [6]. With the ascent of fermion actions which satisfy the Ginsparg-Wilson relation it makes sense to disentangle chirality violation effects from ordinary scaling violation effects, and in a recent paper A. Hasenfratz has shown some evidence [5] that one should primarily suspect the former type of discretization effects to give rise to the excessive $\Sigma$ values listed in Table 1.

**Proximity of the “conformal window”:** The more “exotic” view is that the fitted value for $\chi_0(m) \simeq \Sigma m/N_f$ is appropriate for $N_f = 2$ QCD, while the standard phenomenological evaluation – even if it involves (non-strange) pions only – concerns QCD with $3 (2+1)$ light flavours. In this scenario the way $\chi$ depends on $m \ll \Lambda_{\text{QCD}}$ has an $N_f$-dependence beyond the one indicated in (3), i.e. the low-energy constant $\Sigma$ depends (strongly) on $N_f$, e.g. $\Sigma_2 \simeq (450 \text{ MeV})^3$ while $\Sigma_3 \simeq (288 \text{ MeV})^3$. The latter gap could then be interpreted as a hint that the “conformal window” (where, for appropriate $N_f$, one has $\Sigma_{N_f} \ll \Lambda_{\text{QCD}}^3$ and chiral symmetry is primarily broken through higher dimensional condensates) might be “close” – see [6] for a discussion and some references.
FIGURE 3. Schematic representation how discretization effects typically affect topological susceptibility data in full QCD with Wilson-type (left) and staggered (right) sea-quarks, if simulations are run at fixed $\beta$ and fixed $m$, respectively. In either case discretization effects tend to enhance the effective $F_\pi$ or $\Sigma$ (in particular for large lattice spacing $a$) and they reduce the associate $\chi_\infty$ by an amount $\propto a^2$. The lattice susceptibility (6) is the reduced mean of the modified functions (fat dots) and may, for $2 < (M_\pi r_0)^2 < 8$, show little variation with $m$ and lie substantially above the expected continuum curve (black line).

REFINED EVALUATION OF $\Sigma_2$ AND $\chi_\infty$

In the following, I concentrate on the first alternative and show that – in the absence of data suitable for a continuum extrapolation – basic knowledge regarding the dominant discretization effects allows for a more sophisticated evaluation of the parameters in (5).

The key observation on which this analysis relies is that the leading lattice artefacts in both elements of (5) – the chiral piece (3) and the quenched piece (4) – are known: On the chiral side the dominant effect is chirality violation (for a discussion see [5, 2]), i.e. $F_\pi r_0 = F_\pi r_0 (1 + \text{const} (a/r_0)^p)$ with $p$ reflecting the fermion formulation. On the quenched side scaling violations are known to result in $\chi_\infty r_0^4 = \chi_\infty r_0^4 - 0.208 (a/r_0)^2$ (with a known coefficient !) [2, 1]. Combining all the ingredients, one ends up with

$$\hat{\chi}_0^4 = 1/\left\{ 2N_f/[(M_\pi r_0)^2(F_\pi r_0)^2(1+\text{const}(a/r_0)^p)^q] + 1/\left[\chi_\infty r_0^4 - 0.208 (a/r_0)^2 \right] \right\},$$

where $q$ may be chosen between 1 and 2, since $(1+O(a^p))^2 = 1+O(a^p)$; I use $q=2$. A qualitative picture how these modifications affect the measured topological susceptibility is drawn in Fig. 3. In this respect it is important to know that in a series of full QCD
simulations at fixed $\beta$ the lattice spacing will *shrink* if the (sea-)quark mass gets reduced (which is often the case in studies with Wilson-type sea-quarks; the only exception is the one by UKQCD, where $\beta$ gets relaxed when $\kappa$ is increased in such a way that $a$ stays approximately constant), whereas if one works in a staggered formulation at fixed quark mass $\hat{m}$ the lattice will get *coarser* as one approaches the chiral limit – eventually the measure resembles more that of a theory with a single pseudo-Goldstone rather than one with $N_f^2 - 1$ pion type degrees of freedom as in the continuum [5].

In order to make use of this knowledge (i.e. to utilize (5) to fit the data) one has to decide on the parameters ($p$, const) showing up in (6). The former choice is relatively easy – I take $p_{\text{CP-PACS}} = 1.5$, $p_{\text{UKQCD}} = 2$, $p_{\text{SESAM}} = 1$, $p_{\text{PISA}} = p_{\text{BOULDER}} = 2$ to account for the formulation and the different strategies regarding $c_{\text{SW}}$. The latter choice – which value “const” shall be given – is more delicate: Ideally, one would like to determine it directly from the data. However, it turns out that the quality of the data at hand is not sufficient to allow for an additional (i.e. third) fitting parameter. A reasonable option would be to determine it from conventional $F_\pi$ measurements on the individual ensembles. A simpler option is to use (6) twice – in a first round “const” is given a likely value by fitting it while $((F_\pi r_0)^2/4, \chi_\infty r_0^4)$ is held fixed at $(0.014, 0.066)$; in a second round the latter get adjusted while “const” is kept fixed at the previously determined value. Obviously, with this simpler option the final outcome for $((F_\pi r_0)^2/4, \chi_\infty r_0^4)$ reflects, to some extent,
TABLE 2. Refined determination of $\Sigma$ and $\chi_\infty$ from full QCD vacuum data with (6), using $r_0 = 0.5$ fm and the GOR-relation to convert to physical units. For a cautionary statement regarding the fitting procedure see text.

|                  | CP-PACS | UKQCD | SESAM | PISA   | BOULDER |
|------------------|---------|-------|-------|--------|---------|
| $(F_\pi r_0)^2/4$| 0.0174  | 0.0134| 0.0299| 0.0340 | 0.0106  |
| $F_\pi$ [MeV]    | 104.    | 91.   | 137.  | 146.   | 81.     |
| $\Sigma^{1/3}$ [MeV] | 311.   | 284.  | 372.  | 388.   | 263.    |
| $\chi_\infty r_0^4$ | 0.0737 | 0.0845| 0.0661| 0.0562 | 0.1466  |
| $\chi_\infty^{1/4}$ [MeV] | 206.  | 213.  | 200.  | 192.   | 244.    |

the corresponding initial values. The simplest option is just to set “const” to a generic value like 1. My personal choice is to take the arithmetic average of the “const” values suggested by the last two options and to use that value to fit for $(F_\pi r_0)^2/4$ and $\chi_\infty r_0^4$.

The result of this exercise is shown in Table 2 and Fig. 4, where dotted lines represent the lattice curve (6) with $(F_\pi r_0)^2/4$ and $\chi_\infty r_0^4$ adjusted such as to make it go through the data points while full lines indicate the associate continuum curve (5). The data in Table 2 should be taken with a grain of salt since, as explained above, there is a remnant trace of the initial values in the final fitting parameters $(F_\pi r_0)^2/4$ and $\chi_\infty r_0^4$. Nonetheless, the result is interesting because it supports the standard view that QCD with $N_f = 2$ is not in the “conformal window” and that its low-energy structure agrees with that suggested by phenomenological investigations in “real” (2+1 flavour) QCD [9], i.e. at least for $N_f = 2$ chiral symmetry is predominantly broken through a distinctively nonzero condensate (for references to an alternative scenario see [6]) and $\Sigma_2$ as suggested by Table 2 is compatible with the value from the GOR-relation, $\Sigma_{2+1} \simeq (288\text{ MeV})^3$.

From a lattice perspective it reassuring to see that through a simple ansatz for the dominant discretization effects today’s state-of-the-art simulations (which, from a naive perspective, seemed to support an almost flat topological susceptibility curve and hence to reproduce – in spite of all unquenching efforts – a more or less quenched vacuum structure) may, in fact, be shown to give supportive evidence in favour of a decreased topological susceptibility near the chiral limit and hence “bear” the knowledge of the difference between the quenched and the unquenched vacuum structure in them. The ultimate goal is, of course, to make discretization effects sufficiently small so that the expected continuum pattern of the vacuum structure gets visible in the raw data already.

REFERENCES

1. A. Ali Khan et al. [CP-PACS collab.], hep-lat/0106010 (2001).
2. A. Hart and M. Teper [UKQCD collab.], hep-lat/0108006 (2001).
3. G. Bali et al. [SESAM/TXL collab.], Phys. Rev. D, 64, 054502 (2001).
4. B. Allés et al. [PISA group], Phys. Lett. B, 483, 139 (2000).
5. A. Hasenfratz, hep-lat/0104015 (2001).
6. S. Dürr, hep-lat/0103011_v2, to appear in Nucl. Phys. B (2001).
7. H. Leutwyler and A. Smilga, Phys. Rev. D, 46, 5607 (1992).
8. A. Ali Khan et al. [CP-PACS collab.], Phys. Rev. Lett., 85, 4674 (2000).
9. G. Colangelo, J. Gasser and H. Leutwyler, Phys. Rev. Lett., 86, 5008 (2001).