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TOWARDS THE TOPOLOGICAL SUSCEPTIBILITY WITH OVERLAP FERMIONS

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Abstract. Using a reweighting technique combined with a low-mode truncation of the fermionic determinant, we estimate the quark-mass dependence of the QCD topological susceptibility with overlap fermions. In contrast to previous lattice simulations which all used non-chiral fermions, our results appear to be consistent with the simple continuum model of Dürr. This indicates that at current lattice spacings the use of the index theorem might not be justified and the fermionic definition of the charge might be needed.

Smooth $SU(3)$ gauge field configurations can be characterised with an integer charge Q, a topological invariant. Topology plays a crucial role in shaping the low-energy behavior of QCD. Instantons are believed to be largely responsible for the spontaneous breaking of chiral symmetry. The axial anomaly [1] as well as the large mass of the η' [2, 3] are also intimately connected to gauge configurations of non-trivial topology. For a good understanding of QCD, it is thus crucial to have a consistent picture of its topological structure.

Fluctuations of the topological charge can be characterised with the topological susceptibility,

$$\chi = \frac{\langle Q^2 \rangle}{V}, \tag{1}$$

where $\langle . \rangle$ denotes averaging with respect to the full QCD measure and V is the volume of the system. One of the most profound effects that light dynamical fermions are expected to have on the QCD vacuum is the suppression of fluctuations of the topological charge. Chiral perturbation theory predicts that in the presence of N_f degenerate light fermion flavours

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the susceptibility vanishes with the quark mass as

$$\lim_{m\to 0}\chi = \frac{\Sigma m}{N_f^2} + \mathcal{O}(m^2) = \frac{f_\pi^2 m_\pi^2}{2N_f} + \mathcal{O}(m_\pi^4), \tag{2}$$

where m_π and f_π are the pion mass and decay constant, Σ is the chiral condensate and m is the quark mass [4].

At the other extreme, when the quarks are very heavy, their influence eventually becomes negligible and the susceptibility approaches its quenched value which is known to be $\chi_q = (203 \pm 5\mathrm{MeV})^4$ [5]. Recently it has also been discussed by S. Dürr how the susceptibility is expected to behave for intermediate quark masses [6]. Starting with the observation that besides the light quarks, the unit volume[1] also suppresses higher topological sectors and noting that these two mechanisms are independent, he derived a phenomenological formula for the susceptibility. In terms of the pion mass it reads as

$$\chi(m_\pi) = \left(\frac{2N_f}{m_\pi^2 f_\pi^2} + \frac{1}{\chi_q}\right)^{-1}. \tag{3}$$

Both f_π and χ_q are independently known therefore this formula has no free parameter. While (3) does not come from first principles, it is based on a physically appealing plausible picture. Even if it is not the last word in this subject, it indicates that the susceptibility might substantially deviate from the Leutwyler-Smilga curve already at smaller quark masses than previously expected and it might be strongly suppressed even at moderately heavy quark masses.

Although it is only the quenched topological susceptibility that has an immediate phenomenological interest, being connected to the η' mass through the Witten-Veneziano formula [2, 3], it would also be of considerable interest to check the expected chiral behaviour of the full (unquenched) susceptibility. This is because in the derivation of the Witten-Veneziano formula it is always tacitly assumed that the full susceptibility goes to zero in the chiral limit (see e.g. [7] for a recent discussion on the lattice).

Recently several attempts have been made to check these predictions against numerical simulations on the lattice but the situation is still rather controversial. Some lattice simulations show only very slight or no suppression of topological fluctuations [8, 9, 10]. The latest UKQCD results [11] obtained with improved Wilson fermions agree well with the Leutwyler-Smilga prediction of Eq. (2), even beyond its expected range of validity and the UKQCD susceptibility is still significantly higher than what Dürr's interpolation formula (3) anticipates.

[1] Recall that the susceptibility is defined as the fluctuation of Q *per unit volume*.

To understand why lattice simulations do not show the expected fermionic suppression of the topological susceptibility, let us briefly look at the physical mechanism that leads to this suppression. In the background of a charge Q smooth gauge configuration the Dirac operator D has (at least) $|Q|$ zero eigenvalues for each flavour, due to the Atiyah-Singer index theorem. The quark effective action — obtained after integrating out the fermions — for N_f flavours is proportional to $\det^{N_f}(D+m)$. In the light quark limit the determinant is $\propto m^{|Q|N_f}$ which leads to the suppression of higher Q sectors and thus the topological susceptibility. All this is true for smooth gauge field configurations in the continuum. The situation in lattice simulations however is rather different since lattice Dirac operators in general do not have exact zero eigenvalues and it is not obvious how the index theorem is realised on the lattice.

For a more thorough understanding of what happens on the lattice, we first note that both the Witten-Veneziano formula and the Leutwyler-Smilga relation follow from the flavour singlet axial Ward Identity (WI). A general (Wilson type) lattice fermion action can be written as

$$S(\theta) = \overline{\psi}\left[D^A + e^{i\gamma_5\theta}(W + m_c M) + (m - m_c)M\right]\psi, \tag{4}$$

where D^A is the naive lattice Dirac operator, W is the Wilson term, M the mass term and we already split off the critical mass m_c to account for the non-trivial mixing between the Wilson and the mass term, and the θ-dependence is also included [12]. Using that D^A anticommutes, while the rest of the Dirac operator commutes with γ_5, it is easy to show that the θ-dependence can be transferred to the mass term by a chiral rotation $\psi(x) \to e^{-i\gamma_5\theta/2}\psi(x)$. This also means that in the chiral limit, $m \to m_c$, the action does not depend on θ.

The flavour singlet axial WI can be derived by making a local change of variables $\psi(x) \to e^{-i\gamma_5\alpha(x)}\psi(x)$ in the fermionic path integral and using that the measure is invariant with respect to this. The variation of the different terms in Eq. (4) give rise to the following terms in the WI,

$$\partial_\mu j^5_\mu(x) - 2N_f\, q(x) + 2(m - m_c)N_f\, \overline{\psi}\gamma_5\psi(x) = 0 \tag{5}$$

By integrating this over all space-time, the divergence of the axial current does not give any contribution and we arrive at

$$\mathcal{Q} = -(m - m_c)\mathrm{Tr}\left[\gamma_5 D(m)^{-1}\right], \tag{6}$$

where $\mathcal{Q}$ is the integral of $q(x)$ over space-time. The term $\mathcal{Q}$ that originates from the Wilson term in the action, is usually identified as the topological charge [13]. We would like to emphasise, however that this identification

is based on perturbative arguments that are valid only in the naive continuum limit and might also hold in the proper continuum limit but there is no reason to believe that any charge obtained directly from gauge field observables (e.g. by cooling) is a reasonably good approximation to $\mathcal{Q}$ in practical situations.

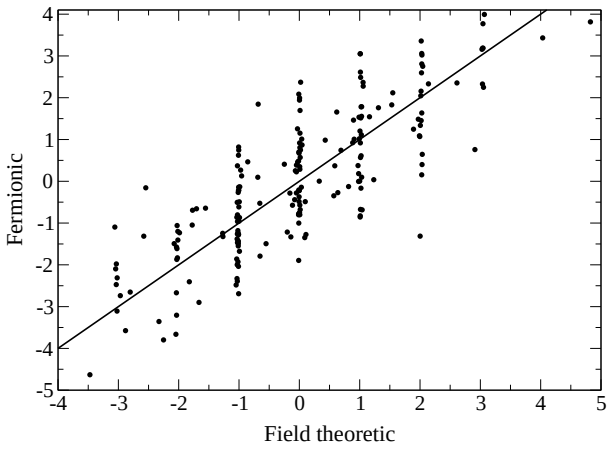

Figure 1. The value of the field theoretic vs. the fermionic charge on a set of $\beta = 5.85$ quenched gauge configurations.

In fact, there is good reason to believe that at current values of the lattice spacing, these quantities are quite different. In Fig. 1 we show a particular field theoretic charge [5] versus $\mathcal{Q}$ on a set of $\beta = 5.85$ quenched configurations[2]. Even though, there is a strong correlation between $\mathcal{Q}$ and the algebraic charge, Q, it is not unlikely that the use of Q instead of the "fermionic" definition $\mathcal{Q}$ can introduce substantial errors.

A possible way to avoid this would be to use the fermionic definition, with the Dirac operator that enters the dynamical simulation. There is even an efficient algorithm to calculate $\mathcal{Q}$ [14] but difficulties emerging in the chiral limit have so far made this approach impracticable.

Recently, through the overlap formulation, it has become possible to put fermions on the lattice while preserving an exact chiral symmetry [15] and avoiding many of the problems other formulations have in the chiral limit. In particular, with the overlap, the above derivation of the WI and the fermionic definition of the charge results in

$$\mathcal{Q} = n_- - n_+, \tag{7}$$

where $n_\pm$ are the number of positive/negative chirality zero modes of D. This makes it possible to define the "topological charge" in a consistent

[2] The $\mathcal{Q}$ values have been slightly rescaled by an overall factor to give the same topological susceptibility as the field theoretic charge.

way avoiding any reference to an algebraic charge that has no a priori connection to the Dirac operator. Another advantage of this formulation is that with chiral fermions the Leutwyler-Smilga relation has been shown to hold exactly in the chiral limit even at finite lattice spacing [16]. This makes chiral fermions extremely suitable for exploring how the topological susceptibility interpolates between the chiral Leutwyler-Smilga and the heavy quark regime.

Unfortunately lattice simulations with dynamical overlap fermions have so far been prohibitively expensive. In the present paper we show the results of a qualitative numerical computation of the susceptibility with overlap fermions. As we shall see, the quark-mass dependence of the susceptibility can be estimated with a suitable reweighting of a quenched ensemble. The procedure we propose is to generate an ensemble $\{U_i\}_1^n$ of quenched gauge field configurations with only the pure gauge measure. In principle the topological susceptibility can then be computed by reweighting each configuration with the corresponding fermion determinant,

$$\chi(m) = \frac{1}{V\,Z} \sum_i \mathcal{Q}_i^2 \det{}^{N_f}[D(U_i) + m], \tag{8}$$

where $D(U_i)$ is the Dirac operator and $\mathcal{Q}_i$ is the charge in the background of the gauge configuration U_i. Z is the partition function, i.e. the sum appearing in Eq. (8) without the $\mathcal{Q}_i^2$ factor.

In principle this is a correct procedure, in practice however it is useless since control over the statistical errors is lost exponentially with increasing volume. The crucial observation is that it is only the small eigenvalues of D that are correlated with the topological charge and without any loss, the full determinant can be replaced with a truncation thereof,

$$\det(D + m) \to \prod_{k=1}^{N} (\lambda_k + m), \tag{9}$$

where $\{\lambda_1, \lambda_2, \ldots \lambda_N\}$ are the N smallest magnitude eigenvalues of D.

In Fig. 2 we show the (reweighted) susceptibility as a function of the number of eigenvalues included in the truncation. For heavier quarks, more eigenvalues should be included in the determinant but overall the truncation is clearly a good approximation. It drastically reduces the variation of the determinant within each topological sector and turns out to make the reweighting practicable in a physically useful range of volumes. The upshot is that once the lowest N eigenvalues of D are known on an ensemble of quenched gauge configurations, the full quark-mass and N_f dependence of the susceptibility can be easily obtained. The only caveat is that for smaller quark mass and larger N_f the determinant fluctuates more and consequently the errors increase.

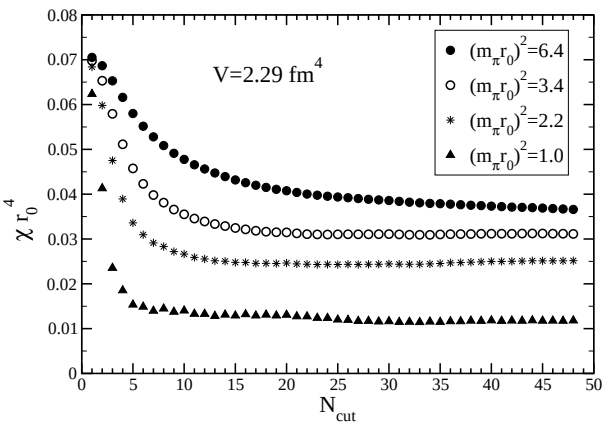

Figure 2. The reweighted topological susceptibility in a $V = 2.29\,\mathrm{fm}^4$ box, as a function of the number of eigenvalues included in the truncated determinant. The different curves correspond to different quark (and pion) masses.

We have seen that the truncation of the fermion determinant is a good approximation for the susceptibility but what does it physically mean to truncate the determinant? We would like to argue that it is essentially just another possible action that differs from the untruncated fermion action only by local gauge terms. Indeed, it has been shown that the contribution of the upper part of the spectrum to the fermion action can be well approximated with a linear combination of small Wilson loops [17], i.e. a local gauge action.

Besides the susceptibility, there are two other quantities of interest in our simulation, the lattice spacing (as set by the Sommer scale r_0) and the dependence of the pion mass on the bare quark mass. It is expected that including the truncated determinant will not substantially change r_0 compared to its quenched value, in conventional dynamical simulations most of the change in r_0 originates from the bulk of the upper part of the Dirac spectrum. Therefore, in this qualitative calculation we completely ignore this effect and use the quenched scale. The change in $m_\pi(m_q)$ compared to the quenched one can be estimated using the GMOR and the Banks-Casher relation together with the available low-end of the Dirac spectrum. The setting of the scale and the pion mass are the two weak points of this calculation which might contain uncontrolled effects. This is the reason why this computation should be considered only as a qualitative first estimate and hopefully in the future it will be checked by a full-blown dynamical overlap calculation. We believe, however that even with these caveats, our calculation is still "competitive" with the currently available dynamical calculations that might have other limitations, as we discussed above.

Simulations at several β values and lattice sizes are currently underway.

As an illustration we show results on an ensemble of 2500 $\beta = 5.85$ ($a = 0.123$ fm) lattices with a volume of $V = 2.29$ fm^4. Our overlap action was constructed by inserting the $c_{sw} = 1.0$ clover operator with 10 times APE smeared gauge links [18] into the overlap formula,

$$D_{ov} = 1 - (1 - D_c) \left[(1 - D_c)(1 - D_c)^\dagger \right]^{-\frac{1}{2}} \tag{10}$$

The inverse square root was approximated with Chebyshev polynomials after treating the lowest eight eigenmodes of $(1 - D_c)(1 - D_c)^\dagger$ exactly [19].

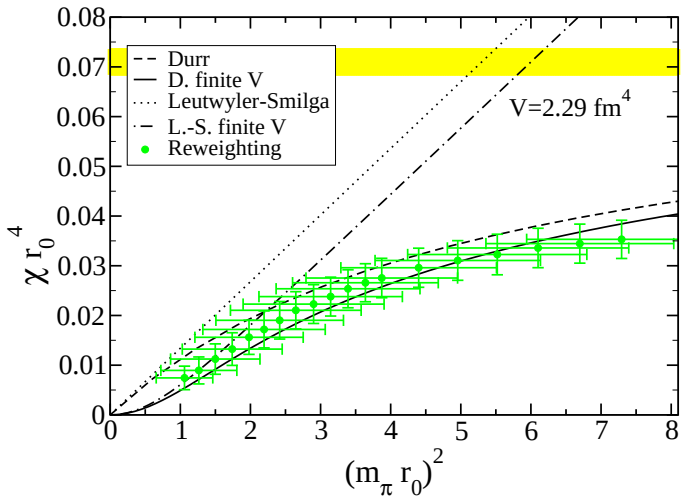

Figure 3. The topological susceptibility vs. pion mass in a box volume of $V = 2.29$ fm^4.

In Fig. 3 we present the main result of this paper, the susceptibility versus the pion mass with $N_f = 2$ flavours of overlap fermions. Both the susceptibility and the pion mass are translated into dimensionless units with the help of the Sommer scale $r_0 = 0.49$ fm [20]. The shaded region indicates the quenched susceptibility $r_0^4 \chi_q = 0.0703(19)$. obtained on the same ensemble without any reweighting. The quoted error is only statistical, we did not include any additional uncertainty coming from the scale setting. In more conventional physical units this translates into $\chi_q = (207.0(1.4)\mathrm{MeV})^4$.

For comparison we also plotted the Leutwyler-Smilga formula and Dürr's formula of Eq. (3) using our measured quenched susceptibility and the known value $f_\pi = 93$ MeV. Since both Eq. (3) and (2) are valid in the infinite volume limit and our volume is not particularly big, we also plotted the curves corresponding to our volume.

In conclusion, we argued that current computations of the topological susceptibility with dynamical quarks might suffer from a systematic error

essentially due to the lack of the index theorem at currently used lattice spacings. We presented a pilot study of the unquenched topological susceptibility with $N_f = 2$ flavours of overlap fermions using reweighting. Our computation involved some uncontrolled approximations for setting the scale and the pion mass which eventually have to be checked in a full-fledged dynamical simulation. Nevertheless, our results appear to be consistent with Dürr's formula and indicate that the susceptibility might be more strongly suppressed than other lattice simulations suggest. It would also be interesting to compute the susceptibility with non-chiral Wilson fermions using the corresponding fermionic definition of the charge.

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