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Topological susceptibility and chiral condensate with $N_f = 2+1+1$ dynamical flavors of maximally twisted mass fermions.

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We study the 'spectral projector' method for the computation of the chiral condensate and the topological susceptibility, using $N_f = 2+1+1$ dynamical flavors of maximally twisted mass Wilson fermions. In particular, we perform a study of the quark mass dependence of the chiral condensate Σ and topological susceptibility χ_{top} in the range 270 MeV $< m_\pi <$ 500 MeV and compare our data with analytical predictions. In addition, we compute χ_{top} in the quenched approximation where we match the lattice spacing to the $N_f = 2+1+1$ dynamical simulations. Using the Kaon, η and η' meson masses computed on the $N_f = 2+1+1$ ensembles, we then perform a preliminary test of the Witten-Veneziano relation.

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1. Introduction

The Banks-Casher relation [1] connects the chiral condensate Σ with the density of eigenmodes at the origin of the spectrum and thus with the infrared properties of the Dirac operator. The chiral condensate is obtained from the eigenvalue density $\rho(\lambda, m)$ in a triple limit, sending the volume V to infinity and the quark mass m as well as the eigenvalues λ to zero (in this order),

$$\frac{\Sigma}{\pi} = \lim_{\lambda \to 0} \lim_{m \to 0} \lim_{V \to \infty} \rho(\lambda, m). \tag{1.1}$$

Only when the eigenvalue density $\rho(\lambda, m)$ is non-zero at the origin, the chiral condensate does not vanish and hence the infrared properties of the Dirac operator are directly related to the mechanism of chiral symmetry breaking.

One way to express $\rho(\lambda, m)$ is through the mode number $\nu(M, m)$, which is defined as the number of eigenmodes λ of the considered Dirac operator squared below some cut-off mass M,

$$\nu(M, m) = V \int_{-\Lambda}^{\Lambda} d\lambda \rho(\lambda, m), \qquad \Lambda = \sqrt{M^2 - m^2}. \tag{1.2}$$

The above considerations can –in principle– be taken over directly to the lattice as a way to compute the chiral condensate non-perturbatively. However, counting the eigenmodes below the cut-off M with $M \approx O(100)$MeV and taking the continuum limit more and more modes have to be taken into account for a fixed physical value of M. In fact, a direct counting of the low-lying eigenmodes is expected to show an $O(V^2)$ scaling behaviour and becomes prohibitively computer time expensive when the continuum limit is taken.

Recently, however, a new method [2] to compute the mode number was developed, the so-called spectral projector method. The important advantage of this method is that it is computationally much faster than counting eigenmodes directly and scales only with the volume V. In addition, the concept of spectral projectors can be extended to evaluations of other quantities such as the topological susceptibility χ_{top} or the ratio of the pseudoscalar and scalar renormalization constants $\frac{Z_P}{Z_S}$, as explained in refs. [2, 3].

It goes beyond the scope of this proceedings contribution to detail the spectral projector method and we have to refer to refs. [2, 3] for a description of this method. The aim of this contribution is rather to see, how the spectral projector method works for computing the chiral condensate and the topological susceptibility in the case of the here used maximally twisted mass fermions formulation of lattice QCD [4]. In particular, in this work we are interested in the quark mass dependence of the chiral condensate and the topological susceptibility and we will work at only one value of the lattice spacing of $a \approx 0.0782$ fm. All results are shown for a setup employing a mass-degenerate light quark doublet and a strange and a charm quark close to their physical values, a situation we refer to as $N_f = 2+1+1$, see refs. [5, 6, 7] for simulation and analysis details. Employing several values of the quark mass will allow us to confront our data with predictions of chiral perturbation theory and to extract values for the chiral condensate in the chiral limit. We will also perform a first test of the Witten-Veneziano formula [8, 9] in this proceedings contribution by computing Kaon, η and η' masses on our dynamical $N_f = 2+1+1$ configurations and the topological susceptibility in the infinite quark mass limit (quenched approximation) matched, however, to the physical situation of the unquenched simulations.

2. Evaluation of the chiral condensate and topological susceptibility

When computing the chiral condensate from spectral projectors, there are two important ingredients. The first is a technical aspect: the spectral projectors are calculated from a stochastic estimate of the "inverse" of some suitable function of the lattice Dirac operator employed, see ref. [2]. Therefore, it needs to be investigated what is a sufficient number of stochastic noise vectors employed and how the stopping criterion for obtaining the solution of a Dirac equation needed to construct the spectral projector. The second aspect is more physical and originates from the fact that the chiral condensate is computed from the slope of the mode number as a function of the cut-off M. Before coming to our results, let us therefore briefly discuss the tests we have made for both issues. In the following, we will use M^* as the cut-off for the mode number counting. M^* is of a very similar size as M and plays the role of an adjustable parameter to optimize the simulations.

As a very first test, we performed a comparison between the explicitly computed mode number and the values from the spectral projectors. In this test we found a perfect agreement demonstrating that our implementation of the spectral projectors in the tmLQCD package [10] is correct.

Looking at the mode number itself as function of M, see fig. 1 (left), we indeed can identify a linear behaviour of the mode number which will allow us in the following to extract the chiral condensate. We also show in fig. 1 (right) our results for changing the number of stochastic sources and the (relative) stopping criterion. As a conclusion from this study we found that with already 6 stochastic sources the corresponding error saturates, nevertheless we used 8 sources to remain safe. In addition, we found that the stopping criterion can be chosen rather loosely and even a choice of 10^{-2} gave completely consistent results. Nevertheless, for our work we decided to choose a stopping criterion of 10^{-6} to be on the safe side.

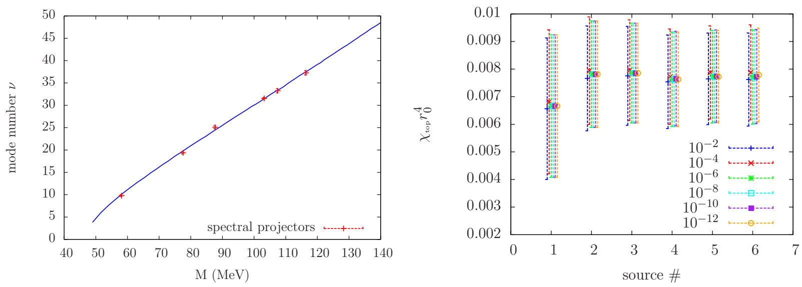

Figure 1: (left) The mode number as a function of M – from explicit computation of eigenmodes (line) and from spectral projectors (points). (right) The influence of the number of stochastic sources and relative precision of solving the Dirac equation.

2.1 Results

After the tests described in the previous section, we proceeded to compute the mode number from spectral projectors. As said above, for this work we used only one value of the lattice spacing of $a \approx 0.0782$fm corresponding to $\beta = 1.95$, as determined by ETMC [6]. While working here only at one value of the lattice spacing, we have computed the mode number at several values of the quark mass, see tab. 1, where we give the bare light twisted mass parameter in lattice units, as well as the pion mass. Note that for all the parameters shown in tab. 1 the theory was tuned to maximal twist. Our typical statistics for computing the mode number and the topological susceptibility has been 200 configurations that were separated by 20 HMC trajectories.

β	lattice	$a\mu_l$	M_π (MeV)
1.95	$32^3 \times 64$	0.0025	270
1.95	$32^3 \times 64$	0.0035	320
1.95	$32^3 \times 64$	0.0055	390
1.95	$32^3 \times 64$	0.0075	455
1.95	$24^3 \times 48$	0.0085	490

Table 1: Parameters of ensembles used to computed the mode number and the topological susceptibility. We give the light bare twisted mass parameter $a\mu_l$ in lattice units as well as the approximate pion masses. The value of $\beta = 1.95$ yields a a lattice spacing of $a \approx 0.0782$fm, see ref. [6].

2.2 Evaluation of the chiral condensate

We have computed the chiral condensate Σ through a study of the average number of eigenmodes of $D^\dagger D$ with $\lambda < (M^\star)^2$, computed using the spectral projector method.

Once the mode number is computed at several values of $M^\star$, the chiral condensate can be calculated directly from the derivative of the mode number with respect to $M^\star$ [2],

$$\Sigma_R = \frac{\pi}{2V}\sqrt{1-\left(\frac{\mu_{l,R}}{M_R^\star}\right)^2}\,\frac{\partial}{\partial M_R^\star}\nu_R(M_R^\star,\mu_{l,R}). \tag{2.1}$$

In eq. (2.1), $\mu_{l,R}$ and $M_R^\star$ denote the renormalized twisted mass and cut-off parameters. The renormalization constant Z_P ($\overline{\mathrm{MS}}$, $\mu = 2$ GeV) needed for obtaining these renormalized quantities has been computed by ETMC in a dedicated four flavour simulation, see ref. [11]. Since the mode number is renormalization group invariant (i.e. $\nu_R(M_R,\mu_{l,R}) = \nu(M,\mu_l)$) [2], from eq. (2.1) we hence obtain directly the renormalized chiral condensate at a scale that is inherited from Z_P.

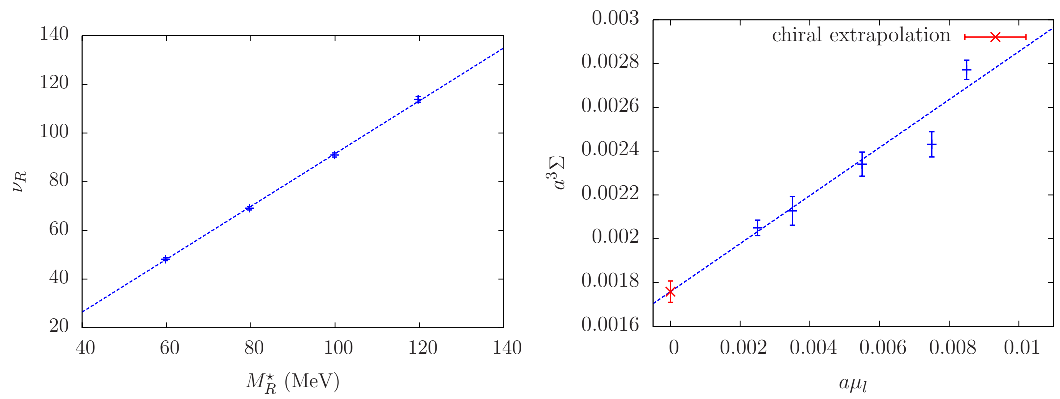

Figure 2: (left) The mode number as a function of $M_R^\star$ for $\mu_{l,R} \approx 14$ MeV and the corresponding linear fit. (right) The chiral condensate Σ_R as a function of the renormalized quark mass. The straight line indicates a linear extrapolation of Σ_R to the chiral limit.

In fig. 2 (left) we show an example of a behaviour of the mode number as a function of $M_R^\star$, for a renormalized quark mass of 14MeV. For the four values of $M_R^\star$ we have used (and similarly as in fig. 1), we observe a linear behaviour of the mode number in the range 60MeV $\lesssim M_R^\star \lesssim$ 120MeV. Such linear behaviour of ν in a range of comparable values of $M_R^\star$ was also observed in ref. [2]. From this linear behaviour, which we see at all five quark masses employed, we can extract the renormalized chiral condensate Σ_R using eq. (2.1) at a given value of the renormalized $M^\star$. In fig. 2 (right) we show as a result the depence of Σ_R on the renormalized quark mass. Extrapolating

Σ_R linearly to the chiral limit, we find $\Sigma_R^{1/3}(\overline{\text{MS}}, \mu = 2\text{GeV}) = 312(1)(13)\text{MeV}$. The first error is purely statistical and the second originates from the uncertainty of the renormalization constant $Z_P(\overline{\text{MS}}, \mu = 2\text{GeV}) = 0.462(13)$ [12].

2.3 Topological Susceptibility

As another quantity accessible to the method of the spectral projectors, we have computed the topological susceptibility χ_{top} following ref. [3]. In this reference it was demonstrated that besides the bare χ_{top} also the renormalized one can be obtained by solely using observables defined through spectral projectors. Since we know the necessary renormalization factor, the ratio of the scalar to the pseudoscalar renormalization constants $\frac{Z_S^2}{Z_P^2}$ available to us from the $N_f = 4$ simulations of ETMC [12], we decided to only compute the bare value of χ_{top} from spectral projectors and to perform the renormalization using the results from ref. [12], i.e. $\frac{Z_P}{Z_S} = 0.685$.

In this way, we have computed χ_{top} at five values of the bare quark mass, listed in tab. 1. Before showing our results, we remark that we have performed a test of the dependence of χ_{top} as a function of the cut-off parameter $M_R^\star$. We found that in the range $90\text{MeV} \lesssim M_R^\star \lesssim 130\text{MeV}$ χ_{top} is constant as a function of $M_R^\star$ and we therefore decided to use a value of $M_R^\star \approx 100\text{MeV}$ for the computation of all subsequent values of χ_{top}.

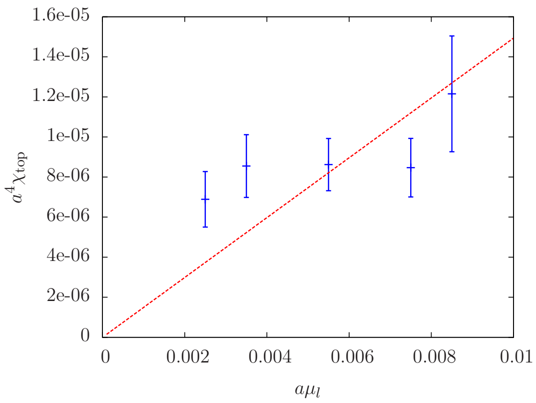

Figure 3: The chiral behaviour of the topological susceptibility with 5 values of the quark mass. The linear fit represents the tree-level formula of χPT, $\chi_{top} = \mu_l\Sigma/2$, and yields a value of the chiral condensate.

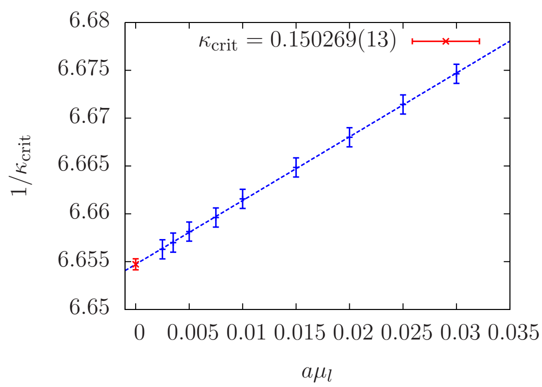

Figure 4: The critical hopping parameter κ_{crit} for the quenched ensemble at $\beta = 2.67$ as a function of μ_l. The linear fit yields the chiral limit value of κ_{crit} which is used to realize maximal twist.

Fig. 3 shows the chiral behaviour of the topological susceptibility. We have fitted our results with the tree-level formula of chiral perturbation theory, $\chi_{top} = \mu_l\Sigma/2$. The fit yields $\Sigma_R^{1/3} = 282(5)(13)$ MeV, where again the systematic error is dominated by the uncertainty in the renormalization constants.

3. Witten-Veneziano formula

As said above, with spectral projectors we have a method at hand that allows for a rather cheap computation of the topological susceptibility, which is, in addition, well defined, i.e. it does not suffer from short distance singularities. Moreover, twisted mass fermions are advantageous for computing disconnected (singlet or OZI) quantities as, e.g., the masses of the η and η' mesons (see the contribution of V. Drach to this conference and refs. [13, 14]).

Thus, it is very tempting to attempt a non-perturbative test of the Witten [8] – Veneziano [9] formula, which provides an elegant explanation for the origin of the unexpectedly large mass of the η' meson. The Witten-Veneziano (WV) formula relates the masses of the Kaon, η and η' mesons to the topological susceptibility χ_∞ where the ∞ index reminds us that the topological susceptibility needs to be computed at infinite quark mass, i.e. in the pure gauge theory. The formula then reads,

$$\frac{f_\pi^2}{4N_f}\left(m_\eta^2 + m_{\eta'}^2 - 2m_K^2\right) = \chi_\infty, \tag{3.1}$$

where f_π is the pion decay constant. Eq. (3.1) cannot be derived in a rigorous way, but some (mild) assumptions are required. It is therefore most worthwhile to test the formula by direct and non-perturbative lattice simulations, since the WV formula is one of the most fundamental relations in QCD and clearly points out the importance of topology.

3.1 Strategy to compute χ_∞

In order to test the WV formula (3.1), the topological susceptibility χ_∞ needs to be computed in the pure gauge theory, but at a matched physical situation. To fulfil this condition, we performed a scan in β using the same (Iwasaki) gauge action as used in [6] and searched for the value of β that gives the same value of the force parameter r_0 as the (chirally extrapolated) one of our dynamical ensembles at $\beta = 1.95$. As a result, we obtained $\beta = 2.67$. The meson masses that are needed in the WV formula were evaluated for a bare twisted mass parameter of $\mu_l = 0.0055$.

Since the topological susceptibility from spectral projectors is a fermionic quantity and we want to use maximally twisted mass fermions, a first step is the tuning to maximal twist. This amounts to tuning the bare Wilson quark mass, or equivalently the hopping parameter κ, to its critical value, m_{crit} , leading to $\kappa_{\text{crit}} = 1/(8+2m_{\text{crit}})$. Following the strategy introduced in ref. [15], we have computed κ_{crit} at different values of the twisted mass μ_l by demanding that the PCAC quark mass vanishes. In the end, we have performed a chiral extrapolation letting μ_l approach zero. Our critical value of κ_{crit} is then the one in the chiral limit. The results of this procedure are shown in fig. 4, which shows that a linear extrapolation to zero twisted mass parameter is justified.

Since in the pure gauge theory and with the Iwasaki gauge action the renormalization constants Z_S and Z_P are not available to us, we decided to follow in this case refs. [2, 3] and compute the renormalized χ_∞ solely from suitable expectation values employing spectral projectors.

In this way, we finally obtained a value of χ_∞ which is listed in tab. 2 together with our results of the meson masses and f_π relevant for the WV formula. Putting everything together and multiplying both sides of eq. (3.1) with r_0^4 to make it dimensionless, we find for the left hand side of the WV formula 0.036(8) and for the right hand side 0.053(18). Although within the errors the WV formula is fulfilled, our present data clearly do not allow us to perform a stringent test.

am_η	$am_{\eta'}$	am_K	af_π	$a^4\chi_\infty$
0.230(10)	0.384(24)	0.2280(4)	0.0656(2)	0.000050(17)
$r_0^4 \frac{f_\pi^2}{4N_f}\left(m_\eta^2 + m_{\eta'}^2 - 2m_K^2\right) = 0.036(8)$				$r_0^4\chi_\infty = 0.053(18)$

Table 2: Results of the meson masses and χ_∞ in pure gauge theory.

4. Conclusion

In this proceedings contribution we have explored the potential of the newly introduced spectral projectors method when applied to maximally twisted mass fermions in the $N_f = 2+1+1$ setup. Our analysis has used only one value of the lattice spacing, but several quark masses which allowed us to compute the chiral condensate in the chiral limit, both from the quark mass dependence of the condensate itself and the topological susceptibility. In addition, we can compare these values to the ones of ref. [6], where the chiral condensate has been extracted from chiral perturbation theory fits to the pion mass and decay constant. In tab. 3 we show these different results. The agreement between the extraction of Σ using very different methods is reassuring.

$\Sigma_R^{1/3}(\mu = 2GeV)[MeV]$		
spectral proj	chiral fits	χ_{top}
312(1)(13)	276(2)(11)	282(5)(13)

Table 3: Results for the chiral condensate obtained with 3 different methods.

As another step, we have performed a first test of the Witten-Veneziano formula. Unfortunately, at the moment our accuracy does not allow for a stringent test of this fundamental relation between meson masses and the (quenched) topological susceptibility. However, the fact that we found reasonable errors already is quite promising that in the future a more precise test can be performed. Clearly, in this work a number of systematic effects could no be considered yet. In particular, it will be interesting to understand the effects of the lattice spacings.

As a last remark, we want to mention that the spectral projector expectation values used to compute the topological susceptibility show a high sensitivity of autocorrelations stemming from topology. Since these expectation values are rather cheap to compute, it can thus be envisaged that such quantities can be used to scrutinize simulations of lattice QCD for possible large autocorrelation times.

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