Topological susceptibility from twisted mass fermions using spectral projectors and the gradient flow

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We compare lattice QCD determinations of topological susceptibility using a gluonic definition from the gradient flow and a fermionic definition from the spectral-projector method. We use ensembles with dynamical light, strange and charm flavors of maximally twisted mass fermions. For both definitions of the susceptibility we employ ensembles at three values of the lattice spacing and several quark masses at each spacing. The data are fitted to chiral perturbation theory predictions with a discretization term to determine the continuum chiral condensate in the massless limit and estimate the overall discretization errors. We find that both approaches lead to compatible results in the continuum limit, but the gluonic ones are much more affected by cutoff effects. This finally yields a much smaller total error in the spectral-projector results. We show that there exists, in principle, a value of the spectral cutoff which would completely eliminate discretization effects in the topological susceptibility.

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I. INTRODUCTION

Topology is essential in understanding the physics of QCD. Due to the fact that the lattice inherently has different topology from the continuum, an accurate and precise measurement of topological charge is a difficult task in lattice QCD, with a long history of failed attempts and practical and theoretical issues to overcome [1–30]. Yet, a good definition of topological charge is essential to modern lattice calculations, e.g. ones involving CP -violation. In particular, the neutron electric dipole moment (nEDM) depends on a topological charge dependent parameter called α^1 , defined in Eq. (31) of [31]. A significant source of error in the nEDM calculation as well as e.g. in the calculation of the mass of the η' meson, is due to uncertainty in the topological charge [32,33].

There are several definitions of topological charge that belong to two broad classes, fermionic and gluonic definitions. In the continuum, it has been widely speculated that they are all equivalent, although it has been rigorously proven only in the quenched theory—in Ref. [34] it has been shown that the cumulants defined from the evolution of the field theoretic topological charge with the Yang-Mills gradient flow (GF) coincide, in the continuum limit, with those of the universal definition appearing in the anomalous chiral Ward identities of QCD. In general, on the lattice different definitions can have very different discretization effects. The gluonic definition, utilizing various smearing techniques to damp UV fluctuations, such as GF [35–37] that we use in this paper, is computationally relatively cheap to calculate and is currently widely used, for example, in the aforementioned nEDM calculation [32]. While computationally cheap, the GF method is known to have large discretization effects [20]. In this paper we focus on a fermionic definition using the method of spectral projectors [16,17], but we also compare the results to ones from a GF-smeared gluonic definition.

Given the topological charge, Q , on every gauge field configuration, the topological susceptibility, χ , is given by the ensemble average $\langle Q^2 \rangle$, divided by the lattice volume V .

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Hence, it is essentially a quantity which provides a measure of topological charge fluctuations. Using leading order chiral perturbation theory (χ PT) and parametrizing the leading discretization term, the topological susceptibility can be written as a simple equation depending on the quark mass and lattice spacing.

In this paper, the coefficient of the mass term, which is a low energy constant (LEC) known as the chiral condensate, Σ , is also extracted, from both the spectral-projector definition and the GF-smeared gluonic definition. Our aim is, in particular, a quantitative investigation of cut-off effects present in both formulations, motivated by our observations that the gluonic topological charge is subject to large discretization effects, at least in the setup of our lattice study (see below).

This paper is organized as follows: Sec. II presents the lattice setup. In Sec. III, we briefly review the spectral-projector method and the gluonic definition of the topological charge (with GF as the smoother), as well as the χ PT formula for topological susceptibility. Section IV contains results from the two methods, together with fits used to determine the continuum value of the chiral condensate. Lastly, we conclude in Sec. V reviewing our results and discussing future directions.

II. LATTICE SETUP

The following calculations were performed using twisted mass configurations with $N_f = 2 + 1 + 1$ dynamical flavors provided by the European Twisted Mass Collaboration (ETMC) [38–40]. The Iwasaki action [41] is used in the gauge sector. The action in the fermionic sector for the light flavors (in the twisted basis) reads: [42–45]

$$S_l = a^4 \sum_x \bar{\chi}_l(x) (D_W + m_0 + i\mu_l \gamma_5 \tau_3) \chi_l(x), \quad (1)$$

where τ^3 is the third Pauli matrix, acting in flavor space, $\chi_l = (\chi_u, \chi_d)$ is a vector in flavor space and D_W is the standard Wilson-Dirac operator. The bare mass parameters, m_0 and μ_l , are the untwisted and twisted light quark masses, respectively. The renormalized light quark mass, which we denote by $\mu_{l,R}$, is related to the bare twisted mass $\mu_{l,R} = Z_P^{-1} \mu_l$, where Z_P is the renormalization function of the pseudoscalar density.

The action for the heavy flavors is [43,45]

$$S_h = a^4 \sum_x \bar{\chi}_h(x) (D_W + m_0 + i\mu_\sigma \gamma_5 \tau_1 + \mu_\delta \tau_3) \chi_h(x), \quad (2)$$

where μ_σ is the bare twisted mass with the twist along the τ_1 direction in charm-strange flavor space and μ_δ gives the splitting along the τ_3 direction, i.e. generates unequal strange and charm quark masses. $\chi_h = (\chi_c, \chi_s)$ is a vector in charm-strange flavor space, written in the twisted basis. The renormalized strange/charm quark masses are combinations of the bare parameters μ_σ and

μ_δ : $\mu_{s/c,R} = Z_P^{-1} (\mu_\sigma \mp (Z_P/Z_S) \mu_\delta)$. Since it is not possible to ideally predict the values of the renormalization functions Z_P and Z_S before a simulation, the renormalized strange/charm quark masses are slightly mistuned with respect to the experimental value, but this effect does not exceed 10% for $\mu_{s,R}$ and 18% for $\mu_{c,R}$ [46]. The effect on topological quantities is expected to be negligible at this level of precision.¹

Twisted mass fermions have the advantage of automatic $\mathcal{O}(a)$ improvement when tuned to maximal twist. Maximal twist is obtained by tuning the hopping parameter, $\kappa = (8 + 2am_0)^{-1}$, to its critical value κ_c , where the PCAC mass vanishes [44,47–50].

Three different lattice spacings were used, ranging from ~ 0.062 – 0.089 fm [46]. For each spacing, we performed calculations for three renormalized quark masses, spanning the interval 12–28 MeV. Topological charge was measured using the gluonic definition on $\mathcal{O}(1000)$ configurations and using the method of spectral projectors on $\mathcal{O}(100$ – $200)$ configurations. Both sets of configurations cover the same range in Monte Carlo time, but the spectral-projector method was used on fewer configurations due to it having greater computational demand. The lattice parameters are collected in Tables I and II, while in Table III we give information on the measurements.

III. THEORY

The method of spectral projectors was introduced and described in detail in Refs. [16,17]. In these papers, the projector was constructed stochastically, thus limiting the computational cost with respect to an explicit computation of eigenmodes from $\mathcal{O}(V^2)$ to $\mathcal{O}(V)$, at the expense of introducing stochastic noise. For the current investigation, we opted for an explicit computation of eigenmodes, in order not to have this stochastic contamination. In practice, we used the ARPACK (ARnoldi PACKage) eigensolver library [53] to calculate the lowest 400 eigenmodes of the normal massless Wilson-Dirac operator, $D_W^\dagger D_W$. We performed the calculations on P100 Nvidia GPU architecture, using the ETMC's code library [54], which uses the QUDA linear solver library as its base [55].

Here, we summarize the relevant details for calculating the topological susceptibility from the Hermitian Wilson-Dirac operator ($D_W^\dagger D_W$) spectrum. The bare topological charge can be defined as

$$Q_0 = \sum_{i, \lambda_i < M_0^2} R_i, \quad R_i = u_i^\dagger \gamma_5 u_i \quad (3)$$

¹In fact, our previous investigation in Ref. [18] showed fully compatible results in $N_f = 2$ and $N_f = 2 + 1 + 1$ setups. Hence, the results are insensitive even to the presence of dynamical strange and charm quarks at the current statistical accuracy.

TABLE I. Parameters of gauge field ensembles, taken from [31,38–40,46,51,52]. Shown parameters are: the inverse bare coupling β , lattice size $(L/a)^3 \times (T/a)$, bare twisted light quark mass μ_l , renormalized quark mass $\mu_{l,R}$, critical value of the hopping parameter, and the number of configurations topological charge was measured on using the gluonic definition (N_{GF}) and the spectral-projector method (N_{spec}). Bolded ensembles were analyzed using only the gluonic definition. In order to have a meaningful comparison, these ensembles are not used in any fits, but they are shown in Figs. 2d–2f.

Ensemble	β	Lattice size	$a\mu_l$	$\mu_{l,R}$ [MeV]	κ_c	N_{GF}	N_{spec}
A30.32	1.90	$32^3 \times 64$	0.0030	12.6	0.163 272	1100	224
A40.24	1.90	$24^3 \times 48$	0.0040	16.8	0.163 270	1125	180
A60.24	1.90	$24^3 \times 48$	0.0060	25.1	0.163 265	1160	212
A80.24	1.90	$24^3 \times 48$	0.0080	33.5	0.163 260	1100	...
A100.24	1.90	$24^3 \times 48$	0.0100	41.9	0.163 255	1018	...
B25.32	1.95	$32^3 \times 64$	0.0025	11.8	0.161 240	971	248
B35.32	1.95	$32^3 \times 64$	0.0035	16.5	0.161 240	1000	201
B55.32	1.95	$32^3 \times 64$	0.0055	26.0	0.161 236	4689	470
B75.32	1.95	$32^3 \times 64$	0.0075	35.5	0.161 232	559	...
B85.24	1.95	$24^3 \times 48$	0.0085	40.2	0.161 231	1128	...
D15.48	2.10	$48^3 \times 96$	0.0015	9.3	0.156 361	646	...
D20.48	2.10	$48^3 \times 96$	0.0020	12.3	0.156 357	1429	94
D30.48	2.10	$48^3 \times 96$	0.0030	18.5	0.156 355	1947	102
D45.32	2.10	$32^3 \times 64$	0.0045	27.8	0.156 315	949	95

and the bare topological susceptibility as

$$\chi_0 = \frac{\langle Q_0^2 \rangle}{V}. \quad (4)$$

The renormalized quantities are

$$\chi = \left(\frac{Z_S}{Z_P} \right)^2 \chi_0, \quad M = Z_P^{-1} M_0. \quad (5)$$

In the above formulas, u_i are eigenvectors of the normal operator $D_W^\dagger D_W$ and M^2 is the renormalized spectral threshold, i.e. all the renormalized eigenvalues taken into account have magnitude smaller than M^2 . The 400 lowest eigenmodes allow M up to 160 MeV for all ensembles described in Table I.

TABLE II. Parameters of gauge field ensembles, common for the same value of β , taken from [31,38–40,46,51,52]. Shown parameters are: β , the lattice spacing a , the Sommer parameter in lattice units r_0/a , the scheme- and scale-independent renormalization functions ratio Z_P/Z_S of the pseudoscalar and scalar densities, and the renormalization function Z_P of the pseudo-scalar density in the $\overline{\text{MS}}$ scheme at the scale of 2 GeV.

β	a [fm]	Z_P	Z_P/Z_S	r_0/a
1.90	0.0885(36)	0.529(9)	0.699(13)	5.231(38)
1.95	0.0815(30)	0.504(5)	0.697(7)	5.710(41)
2.10	0.0619(18)	0.514(3)	0.740(5)	7.538(58)

For chiral fermions, such as overlap fermions, the topological charge receives contributions only from exact zero modes of $D_W^\dagger D_W$. The zero modes correspond to $\lambda = 0$, such that $R_{\lambda=0} = \pm 1$ and $R_{\lambda>0} = 0$. This would indicate that a spectral threshold slightly larger than zero would be enough to obtain a topological charge exactly equivalent to the one from the index of the overlap Dirac operator [56–58]. For non-chiral fermions, such as Wilson

TABLE III. Ensemble label, the step between measurements (in units of molecular dynamics trajectories), integrated autocorrelation time and the relative error of the extracted topological susceptibility. The spectral-projector quantities regard the case of $M = 120$ MeV and are denoted by “spec,” while the gluonic ones are denoted by “GF” and correspond to $t^2 \langle E \rangle = 0.7$. Bolded ensembles were only analyzed using the gluonic definition.

Ensemble	step _{spec}	$\tau_{\text{int,spec}}$	step _{GF}	$\tau_{\text{int,GF}}$	Relative errors	
A30.32	24	0.58	4	1.09	10%	7%
A40.24	20	0.50	4	0.92	11%	6%
A60.24	20	0.53	4	0.73	10%	5%
A80.24	...	...	4	0.79	...	5%
A100.24	...	...	4	0.75	...	5%
B25.32	24	0.49	4	0.72	8%	6%
B35.32	20	0.43	4	1.01	11%	6%
B55.32	20	0.69	2	1.65	8%	4%
B75.32	...	...	4	0.53	...	6%
B85.24	...	...	4	0.80	...	6%
D15.48	...	...	2	1.86	...	12%
D20.48	40	0.67	2	2.20	18%	8%
D30.48	40	0.60	2	5.11	15%	11%
D45.32	40	0.41	4	2.19	13%	11%

twisted mass fermions which we use in this paper, the would-be zero and nonzero modes are shifted by $\mathcal{O}(a^2)$ effects. Moreover, different values of the spectral threshold may correspond to different cut-off effects. An optimal value of M , i.e. one minimizing discretization effects, can be chosen by analyzing several values of the lattice spacing. This allows one to find such a value that the slope of the topological susceptibility vs. the lattice spacing is minimal, as we show explicitly below. The value that we find is appropriate for the here considered setup and it may be different when using e.g. a different fermion discretization. If one works with a single ensemble, it is, of course, not possible to find such an optimal value. However, one can still check the dependence of the topological susceptibility on M and if a region of small variation of the susceptibility is found, it likely corresponds to small cutoff effects, as we also observe in our data. Note that the topological susceptibility from the spectral-projector method is automatically $\mathcal{O}(a)$ -improved when using twisted mass fermions at maximal twist [22].

The other definition of the topological charge that we employ in this paper is the gluonic (field theoretic) one. The calculation of the topological charge with this definition proceeded along the lines of Ref. [24], which we refer to for more details. The field theoretic definition reads:

$$q(x) = \frac{1}{32\pi^2} \epsilon_{\mu\nu\rho\sigma} \text{tr}[G_{\mu\nu}(x)G_{\rho\sigma}(x)],$$

$$Q = a^4 \sum_x q(x), \quad \chi = \frac{\langle Q^2 \rangle}{V}. \quad (6)$$

The definition of the field strength tensor used is tree-level Symanzik improved, i.e. $\mathcal{O}(a^2)$ improved by including both clover terms and rectangular Wilson loops, as described in Ref. [24]. UV fluctuations are filtered using the GF procedure, as described in Ref. [35]. The smoothing action in the GF is the tree-level Symanzik improved gauge action. We looked at different flow times and in the following, we will show results for three flow times, corresponding to $t^2 \langle E \rangle = 0.3, 0.5, 0.7$, where t is the flow time and E is the energy density.

Next, we derive an expression for the topological susceptibility in chiral perturbation theory, following the arguments used in Ref. [59] but adapted for twisted mass. First, we consider the partition function of QCD with nonzero Θ_{QCD} :

$$Z(\Theta) = \int \mathcal{D}A_\mu \mathcal{D}\psi \mathcal{D}\psi^\dagger e^{-S_{\text{QCD}, \Theta=0} + i\Theta Q[A_\mu]}. \quad (7)$$

The topological susceptibility can be written as the second derivative of the energy density, evaluated at $\Theta = 0$,

$$\chi = \left. \frac{\partial^2 \varepsilon(\Theta)}{\partial \Theta^2} \right|_{\Theta=0} = \frac{\langle Q^2 \rangle}{V}, \quad \varepsilon(\Theta) = -\frac{\log(Z)}{V}. \quad (8)$$

The lowest order, two flavor χ PT Lagrangian can be written as:

$$\mathcal{L}_{\chi\text{PT}}^{(2)} = \frac{f_\pi^2}{4} \text{tr}[\partial_\mu U(x) \partial^\mu U(x)^\dagger] - \Sigma \text{Re}(\text{tr}[\mathcal{M} U(x)^\dagger]), \quad (9)$$

where $U(x)$ is an element of $SU(2)$ that can be expressed as $U(x) = \mathbb{1} \cos(\phi(x)) + i\hat{n} \cdot \vec{\tau} \sin(\phi(x))$, where $\hat{n}$ is a unit vector in $\mathfrak{su}(2)$ flavor space. $\mathcal{M}$ is the quark mass matrix, which for two maximally twisted light flavors is just $\mathcal{M} = i\tau_3 \mu_l$. f_π and Σ are low energy constants, identified as the pion decay constant and the chiral condensate, respectively. Θ_{QCD} can be included by using the fact that the physical vacuum angle depends on the argument of the determinant of the quark mass matrix, $\Theta_{\text{phys}} = \Theta + \arg \det(\mathcal{M})$. Thus, a nonzero Θ_{QCD} can be included by rotating it into the mass matrix, $\mathcal{M} \rightarrow \mathcal{M} \tau_3 e^{i\Theta/2}$.

The partition function can now be written in terms of $\mathcal{L}_{\chi\text{PT}}^{(2)}$:

$$Z(\Theta) = \int \mathcal{D}U e^{-\int d^4x \mathcal{L}^{(2)}(U(x), \Theta)}. \quad (10)$$

For volumes that are large relative to the quark mass, $V\mu_l \Sigma \gg 1$, the group integral is dominated by $U(x)$ and by extension $\phi(x)$, which is x independent and minimizes $\mathcal{L}_{\chi\text{PT}}^{(2)}$. For maximal twist and non-zero Θ , this minimum occurs at $\phi = \pm\pi/2$, $\hat{n} = (0, 0, 1)$. The partition function simplifies to: [60–62]

$$Z(\Theta) = Z_0 e^{2V\Sigma\mu_l \cos(\Theta/2)}, \quad (11)$$

which yields:

$$\chi = \left. \frac{\partial^2 \varepsilon(\Theta)}{\partial \Theta^2} \right|_{\Theta=0} = \frac{\Sigma\mu_l}{2}, \quad (12)$$

which is correct to leading order in the quark mass. In the lattice calculation, there will be corrections of order a^2 , as maximal twist removes any $\mathcal{O}(a)$ effects.

IV. EXTRAPOLATION OF THE CHIRAL CONDENSATE

A. Three-parameter fit

One approach for determining the chiral condensate is a global 3-parameter fit to data at different values of the quark masses and the lattice spacing. Specifically, we fit to the expression:

$$r_0^4 \chi = [r_0^3 \Sigma] \frac{r_0 \mu_{l,R}}{2} + [c] \left(\frac{a}{r_0} \right)^2 + \left[\frac{\alpha}{r_0} \right] r_0 \mu_{l,R} \left(\frac{a}{r_0} \right)^2, \quad (13)$$

FIG. 1. Cross sections of global fits of topological susceptibility to the form of Eq. (13) at $a = 0.089, 0.082, 0.062$ fm, shown in plots (a), (b) and (c), respectively. Values labeled with M correspond to the spectral-projector method and with $t^2 \langle E \rangle$ to the gluonic one. Statistical errors are the result of a bootstrap procedure with 1000 samples and appropriate blocking. Note that the values are offset on the horizontal axis for visibility. Ensembles used are summarized in Table I. Resulting fit parameters are shown in Table IV.

where r_0 is the Sommer parameter, used to make all quantities dimensionless, Σ is the renormalized chiral condensate, and c and α are the coefficients of the $\mathcal{O}(a^2)$ and $\mathcal{O}(\mu_l a^2)$ discretization terms. The square brackets indicate the actual fitting parameters. Other expressions were tested, including a two parameter fit, where α was set to zero. Ultimately, the three parameter fit in Eq. (13) was chosen, as it consistently had the smallest χ^2 per degree of freedom for each value of M and $t^2 \langle E \rangle$. Cross sections of the fit at different lattice spacings are shown in Figs. 1(a), 1(b), and 1(c) for three values of M and of $t^2 \langle E \rangle$. The fits themselves, for each of these values of M and $t^2 \langle E \rangle$, are shown in Figs. 2(a), 2(b), 2(c), and 2(d). In Fig. 3 extracted values of $r_0 \Sigma^{1/3}$ are shown for a large range of values of M and for three values of $t^2 \langle E \rangle$. The total discretization coefficient, $[c] + [\alpha/r_0] r_0 \mu_{l,R}$, is shown for three values of $\mu_{l,R}$ in Fig. 4. A summary of the obtained fit parameters is presented in Table IV.

The first observation from Fig. 3 is that a consistent value of $\Sigma^{1/3}$ is obtained for any value of M in the spectral-projector method, with a small tendency for a smaller value for M below around 50 MeV. The values from the gluonic GF definition are essentially independent of the flow time

and consistent with all the spectral-projector values. For spectral projectors, the statistical error noticeably increases for $M \gtrsim 170$ MeV due to fewer ensembles being included in the fits. The statistical error from the spectral-projector definition is a factor of 2–4 smaller than the one from the gluonic definition. This results from the fact that even though we used typically 5 times more configurations for GF, the presence of large cutoff effects in the gluonic definition inflated the error of the final quantity, the chiral condensate, significantly.

The magnitude of discretization effects can be seen in Fig. 4. The spectral-projector definition produces a topological susceptibility with much smaller cutoff effects compared to the gluonic one, regardless of the choice of M and $t^2 \langle E \rangle$. It can be observed that value of M which minimizes discretization effects has some quark mass dependence. For the smallest mass, $\mu_{l,R} = 12.6$ MeV, the optimal value is at ~ 90 MeV (with cutoff effects being compatible with zero in the range 70–120 MeV). For $\mu_{l,R} = 18.5$ MeV, M is optimal at around 120 MeV (compatible with zero for 80–180 MeV). Finally, for the largest mass, $\mu_{l,R} = 26.0$ MeV, M is optimal at ~ 170 MeV (compatible with zero for 80–230 MeV). For the gluonic

FIG. 2. Global fits of topological susceptibility to the form of Eq. (13) for spectral projectors with $M = 80, 120, 160$ MeV and the gluonic definition using gradient flow at flow times $t^2\langle E \rangle = 0.3, 0.5, 0.7$. Statistical errors are the result of a bootstrap procedure with 1000 samples and appropriate blocking. Ensembles used are summarized in Table I. Resulting fit parameters are shown in Table IV. The open points in 2d, 2e, 2f were not included in the fit to make a direct comparison of spectral projectors and GF on the same ensembles.

GF definition, the cutoff effects are basically independent of the flow time. This can be traced back to the fact that the values of the topological susceptibility for single ensembles have very little flow time dependence already after very small flow time, typically of order 0.5 in lattice units, which is roughly an order of magnitude below the flow time corresponding to $t^2\langle E \rangle = 0.3$, which defines the scale referred to as t_0 .

It appears that the spectral-projector method has larger mass-dependent discretization effects compared to the gluonic definition, as α/r_0 has larger magnitude, and smaller mass-independent discretization effects, as c is

smaller. It should be noted, however, that the statistical error in α/r_0 is large enough that the values for both spectral projectors and the gluonic definition are compatible.

It is theoretically justifiable and the above results demonstrate it also numerically that continuum limit results are independent of the spectral threshold M or the flow time. To profit from this fact, we also performed a combined global fit with 5 values of M , 80, 100, 120, 140 and 160 MeV, simultaneously² The correlations between

²We thank Stephan Dürr for suggesting this idea.

FIG. 3. Values of $r_0 \Sigma^{1/3}$ from global fits of topological susceptibility to the form of Eq. (13). Blue (black) points correspond to spectral projectors (GF) and the proper horizontal axis is the lower (upper) one, respectively. Statistical errors are the result of a bootstrap procedure with 1000 samples and appropriate blocking. Ensembles used are summarized in Table I. Resulting fit parameters are shown in Table IV.

topological charges for different values of M were taken into account via a bootstrap procedure, with appropriate blocking to also account for autocorrelations. The resulting global fit had 45 data points and 11 fitting parameters—the M -independent continuum limit chiral condensate and the 10 M -dependent c and α/r_0 fitting parameters describing mass-independent and mass-dependent discretization effects, respectively. We note that when we are including

more values of M , the stability of the fit is lost. In principle, one could further slightly improve the statistical error on the final chiral condensate by including the GF data. However, they were produced with much larger statistics for each ensemble and hence, it is not possible to properly take correlations into account when combining with spectral-projector data. The expected gain from adding the GF data is, anyway, small, which is due to the large discretization effects of this definition.

In the end, we obtained the following value of the chiral condensate from the global spectral-projector fit:

$$r_0 \Sigma^{1/3} = 0.764(30), \quad \Sigma^{1/3} = 318(12) \text{ MeV}, \quad (14)$$

which is a gain of 1/3 in statistical error as compared to a single- M fit for $M = 80$ MeV. We take it as our preferred value for the approach of this subsection.

B. $\chi(a \rightarrow 0)$ LO fit

In order to obtain an estimate of a systematic error resulting from the choice of the ansatz for the fit, we have used a second method for extracting the continuum values of the chiral condensate. While each ensemble used has a different quark mass, each lattice spacing has a small, medium, and large quark mass ensemble. First, we choose one representative small, medium, and large quark mass

FIG. 4. Total discretization error from fitting to the form Eq. (13) for $\mu_{l,R} = 12.6, 18.5, 26.0$ MeV. Blue (black) points correspond to spectral projectors (GF) and the proper horizontal axis is the lower (upper) one, respectively. Error bars are the result of 1000 bootstrap samples for each ensemble. Ensembles used are summarized in Table I and II. Fit parameters are shown in Table IV.

TABLE IV. Fit parameters from Eq. (13) and quality of the fit, $\chi^2/\text{d.o.f.}$. Gradient flow results are labeled with “GF” and a value of $t^2\langle E \rangle$. Spectral projector results are labeled with “SP”: $M = 80$ –160 MeV are global fits using all ensembles in Table I (apart from the ones in bold font); $M = 200$ MeV excludes ensembles A30.32, D20.48, and D30.48, as 400 eigenmodes were not enough to reach $M = 200$ MeV for these ensembles. SP “combined” is the result of a combined global fit with 5 values of M , 80, 100, 120, 140 and 160 MeV, simultaneously, taking correlations (and autocorrelations) into account with a bootstrap procedure (1000 samples and appropriate blocking; used also for single- M fits and all GF fits).

Method	M [MeV]/ $t^2\langle E \rangle$	$\Sigma^{1/3}$ [MeV]	$r_0\Sigma^{1/3}$	c	α/r_0	N_{ens}	$\chi^2/\text{d.o.f.}$
SP	80	316(18)	0.760(44)	0.121(32)	−4.7(1.4)	9	0.281
SP	120	318(21)	0.764(50)	0.191(46)	−4.6(1.8)	9	0.233
SP	160	318(23)	0.764(55)	0.249(54)	−4.3(2.0)	9	0.198
SP	200	318(30)	0.764(73)	0.291(60)	−3.9(2.5)	6	0.066
SP	combined	318(12)	0.764(30)	...	...	9	0.108
GF	0.3	303(44)	0.73(11)	1.15(12)	0.3 (3.8)	9	0.348
GF	0.5	296(47)	0.71(11)	1.18(12)	−0.2(3.9)	9	0.278
GF	0.7	289(49)	0.69(12)	1.15(12)	0.7(3.8)	9	0.261

and find the comparable values of topological susceptibility for each lattice spacing by performing a small linear interpolation to the same mass. For example, for the small quark mass, we choose $\mu_{l,R} = 12.6$ MeV, which is the mass of the A30.32 ensemble, seen in Table I. For the B ensembles, for which $a \approx 0.082$ fm, the $\mu_{l,R} = 12.6$ MeV topological susceptibility was found by linearly interpolating between the B25.32 and B35.32 values, 12.3 MeV and 18.5 MeV, respectively.

The continuum limit of the topological susceptibility is taken for these three masses and obtained by performing a fit linear in $(a/r_0)^2$, using the ansatz:

$$r_0^4\chi(a) = [K](a/r_0)^2 + [r_0^4\chi(a=0)], \quad (15)$$

where $r_0^4\chi(a=0)$ is the continuum value of the susceptibility. The square brackets again denote the actual fit parameters. The extracted values of the susceptibility can be found in Table V.

The results of this procedure are collected in Figs. 5(a), 5(b), and 5(c), for the small, medium, and large quark masses, respectively. A comparison of the discretization effects, contained in the parameter K , is shown for a range of values of M and $t^2\langle E \rangle$ in Fig. 7.

To calculate the chiral condensate, each extracted continuum value of the topological susceptibility is plotted against the quark mass and fitted to the continuum lowest order χ PT formula, Eq. (12), or in dimensionless form:

$$r_0^4\chi(a=0) = [r_0^3\Sigma] \frac{r_0\mu_{l,R}}{2}. \quad (16)$$

This fit is shown in Fig. 6 and the corresponding values of the renormalized chiral condensate are presented in Table VI.

From Figs. 5(a), 5(b), and 5(c), it is apparent that for a given quark mass all values of M and $t^2\langle E \rangle$ converge to the same value in the continuum limit, within errors. This is as

expected, as the definitions should only differ at finite lattice spacing.

We observe that the spectral-projector definition produces a topological susceptibility with much smaller discretization effects compared to the gluonic one, regardless of the choice of M and $t^2\langle E \rangle$. From Fig. 7 the optimal choice of M in order to minimize discretization effects can be concluded. For all considered renormalized quark masses, cutoff effects are compatible with zero in the interval between 100–120 and at least 160 MeV. This range is consistent with the one found from the global fit method, with some tendency of pointing to slightly larger values of

TABLE V. Fit parameters from Eq. (15) using ensembles from Table I. Values from spectral projectors are labeled with “SP” and an M value. Values from the gradient flow are labeled with “GF” and a value of $t^2\langle E \rangle$. Statistical errors are the result of 1000 bootstrap samples for each ensemble.

$\mu_{l,R}$ [MeV]	method	M [MeV]/ $t^2\langle E \rangle$	$r_0^4\chi(a=0)$	K
12.6	SP	80	0.0088(16)	−0.084(48)
12.6	SP	120	0.0093(20)	−0.020(62)
12.6	SP	160	0.0096(23)	0.032(71)
12.6	GF	0.3	0.0065(37)	1.18(13)
12.6	GF	0.5	0.0066(37)	1.18(13)
12.6	GF	0.7	0.0075(38)	1.11(13)
18.5	SP	80	0.0120(13)	−0.166(48)
18.5	SP	120	0.0121(15)	−0.079(60)
18.5	SP	160	0.0118(16)	−0.003(68)
18.5	GF	0.3	0.0094(28)	1.10(13)
18.5	GF	0.5	0.0088(27)	1.11(13)
18.5	GF	0.7	0.0088(28)	1.10(13)
26.0	SP	80	0.0143(24)	−0.191(77)
26.0	SP	120	0.0151(29)	−0.124(94)
26.0	SP	160	0.0147(32)	−0.05(10)
26.0	GF	0.3	0.0137(58)	1.12(19)
26.0	GF	0.5	0.0114(59)	1.18(19)
26.0	GF	0.7	0.0101(60)	1.22(20)

FIG. 5. Continuum extrapolations at $\mu_{l,R} = 12.6, 18.5, 26.0$ MeV, respectively. The actual calculated value of the topological susceptibility was used for the largest lattice spacing, the other two were generated by a linear interpolation of results from the ensembles with the two nearest quark masses. Statistical errors are the result of a bootstrap procedure with 1000 samples and appropriate blocking. Ensembles used are summarized in Table I.

M and with smaller quark mass dependence. Regardless of the method used, the spectral-projector method for any M has significantly smaller discretization effects compared to the gluonic definition at any flow time, not only the considered $t^2\langle E \rangle$ values, but also extending down to approx. 10 times smaller flow times and, presumably, also for larger

ones, because of clear plateaus in (single-ensemble) topological susceptibilities as a function of the flow time.

The fit values of $r_0\Sigma^{1/3}$ seen in Table VI are larger but within errors of the values found using the global fit (cf. Table IV). The statistical errors are smaller, likely due to being more constrained, only fitting to one parameter. However, the χ^2 per degree of freedom is larger for the spectral projectors results, for which reason we prefer the values from the global fit.

FIG. 6. Continuum fit to the lowest order χ PT expression for topological susceptibility, Eq. (16). Values are the continuum extrapolated ones seen in Figs. 5(a), 5(b), and 5(c). Statistical errors are the result of a bootstrap procedure with 1000 samples and appropriate blocking. Note that the values are offset on the horizontal axis for visibility (the true values of $\mu_{l,R}$ correspond to black points).

TABLE VI. Values of the renormalized chiral condensate, from fits of Eq. (16) and quality of the fit, $\chi^2/\text{d.o.f.}$. Values from spectral projectors are labeled with “SP” and an M value. Values from the gradient flow are labeled with “GF” and a value of $t^2\langle E \rangle$. Statistical errors are the result of a bootstrap procedure with 1000 samples and appropriate blocking.

Method	M [MeV]/ $t^2\langle E \rangle$	$\Sigma^{1/3}$ [MeV]	$r_0\Sigma^{1/3}$	$\chi^2/\text{d.o.f.}$
SP	80	336(10)	0.807(23)	0.555
SP	120	339(11)	0.815(26)	0.344
SP	160	337(12)	0.809(29)	0.387
GF	0.3	317(24)	0.761(58)	0.008
GF	0.5	309(25)	0.742(60)	0.034
GF	0.7	308(26)	0.740(62)	0.171

FIG. 7. Total discretization error from a fit to the form of Eq. (15) for $\mu_{LR} = 12.6, 18.5, 26.0$ MeV, in the plots (a)–(c), respectively. Blue (black) points correspond to spectral projectors (GF) and the proper horizontal axis is the lower (upper) one, respectively. Statistical errors are the result of a bootstrap procedure with 1000 samples and appropriate blocking. Ensembles used are summarized in Table I. The resulting fit parameter, K , is shown in Table V.

V. CONCLUSIONS

In this paper, we have compared the calculation of the topological susceptibility and the chiral condensate using the spectral-projector method to an $\mathcal{O}(a^2)$ -improved gluonic definition using the gradient flow. The topological susceptibility computed using spectral projectors was found to have much smaller discretization effects in the considered setup. It should be noted, however, that in the case of the gradient flow an improved definition could be derived which reduces cutoff effects significantly [63,64]. It would therefore be interesting whether such an improved definition can also be found for the here considered topological susceptibility. We have also determined that a spectral cutoff as small as $M \sim 50$ MeV is sufficient for extracting fit quantities, such as the chiral condensate. The optimal choice of M which minimizes discretization effects depends on the details of the ensemble, specifically the quark mass, with lighter masses corresponding to smaller M . In this investigation, we see from Fig. 3 that our choice of M has little effect on $r_0\Sigma^{1/3}$, as long as discretization effects are understood and parametrized. For citing a value, we use the combined global fit value from $M = 80, 100, 120, 140, 160$ MeV (see Table IV) as the central value and the difference with respect to the result from the continuum extrapolated susceptibility (Table VI) as an estimate of the systematic error:

$$r_0\Sigma^{1/3} = 0.764(30)_{\text{stat}}(51)_{\text{sys}},$$

$$\Sigma^{1/3} = 318(12)_{\text{stat}}(21)_{\text{sys}} \text{ MeV}, \quad (17)$$

where we have used $r_0 = 0.474$ fm [46] to convert to physical units. Comparing to our previously calculated values, this result is slightly larger. One value, $r_0\Sigma^{1/3} = 0.651(61)$ [18] is from a fit of the leading order χ PT to the quark mass dependence of the topological susceptibility evaluated with stochastic spectral projectors on a similar set of ensembles. Another, $r_0\Sigma^{1/3} = 0.689(16)(29)$ [65] resulted from direct extraction of the condensate from the mode number evaluated also with stochastic spectral projectors on a similar set of ensembles. While slightly larger, this result is still compatible within errors.

By choosing an appropriate value of M , we have shown the method of spectral projectors eliminates discretization artifacts in topological susceptibility up to our computed precision. This is highly relevant for calculating topological charge dependent quantities, when there is only one lattice spacing available and a continuum extrapolation cannot be performed. This is at present the case with the physical point ensembles recently generated by the ETMC [66–68]. We believe that this approach will significantly reduce discretization errors due to the topological charge, while preserving reasonable statistical errors, allowing more accurate computation of experimentally relevant physical parameters.

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