On the chiral anomaly and the Yang–Mills gradient flow

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Abstract

There are currently two singularity-free universal expressions for the topological susceptibility in QCD, one based on the Yang–Mills gradient flow and the other on density-chain correlation functions. While the latter link the susceptibility to the anomalous chiral Ward identities, the gradient flow permits the emergence of the topological sectors in lattice QCD to be understood. Here the two expressions are shown to coincide in the continuum theory, for any number of quark flavours in the range where the theory is asymptotically free.

1. The usefulness of the Yang–Mills gradient flow in QCD largely rests on the still somewhat surprising fact that it does not require renormalization [1-3]. In particular, correlation functions of local gauge-invariant fields built from the gauge field, such as the Yang–Mills action density $s(t,x)$ and the topological charge density $q(t,x)$, are finite and have no short-distance singularities if evaluated at positive gradient-flow time $t$.

An early application of the flow showed that the field space in a finite space-time volume $V$ dynamically divides into disconnected sectors of fixed topological charge

$$Q_t = \int d^4 x q(t,x)$$

(1)

in the continuum limit of lattice QCD [1]. Moreover, as long as $t > 0$, the sectors are independent of the flow time and so is the topological susceptibility $\chi^{fl}_t = \langle Q_t^2 \rangle / V$. The expression provides a regularization-independent definition of the susceptibility,
which is close to its naive definition, but properly deals with the fluctuations of the gauge field and the associated ultraviolet singularities.

Other singularity-free expressions for the susceptibility, the so-called \textit{density-chain formulae}, have previously been derived using a combination of chiral Ward identities [4] or the index theorem [5]. A diagonal quark mass matrix $M$ is assumed in this case, with positive entries $m_1, m_2, \ldots$ on the diagonal, and the susceptibility is represented through correlation functions like [5]

$$
\chi^\text{dc}_t = m_1 \ldots m_5 \int d^4 x_1 \ldots d^4 x_5 \langle P_{12}(x_1)S_{23}(x_2)S_{31}(x_3)P_{45}(x_4)S_{54}(0) \rangle \tag{2}
$$

of the scalar and pseudo-scalar quark densities $S_{rs}(x)$ and $P_{rs}(x)$ with flavour indices $r, s$ chosen in a particular way. Equation (2) involves five flavours of quarks, which can be valence quarks, if the theory includes a smaller number of sea quarks.

2. The gradient-flow and the density-chain expression for the topological susceptibility, $\chi^\text{fl}_t$ and $\chi^\text{dc}_t$, are both well defined and unambiguously normalized, but they refer to different aspects of the theory, the first characterizing the distribution of the topological charge $Q_t$ in the functional integral, while the second derives from an essentially algebraic property of the theory (the anomalous chiral symmetry). So far their equality has been proved in the pure SU($N$) gauge theory [6] and numerical simulations suggest that the expressions coincide in QCD with non-zero numbers of sea quarks too [7].

In this letter, the equality of the two expressions is first established assuming the number $N_f$ of sea quarks is at least 5 and such that asymptotic freedom is not lost. The theory with fewer flavours of sea quarks is then briefly discussed in sect. 7. As an intermediate regularization of the theory, a formulation of lattice QCD is chosen (the same as in ref. [5]), which preserves chiral symmetry [8-14]. Since $\chi^\text{fl}_t$ and $\chi^\text{dc}_t$ are both regularization-independent, the details of the intermediate regularization are irrelevant, but the argumentation becomes particularly transparent with this choice of regularization. The existence of the continuum limit at the non-perturbative level and the validity of the general principles of renormalization are however taken for granted.

Although the quark mass matrix $M$ is eventually set to a positive diagonal matrix, it is initially taken to be a general complex matrix. In the formal continuum theory, the quark action is then

$$
S_F = \int d^4 x \overline{\psi}(x) \left\{ \not{D} + MP_- + M^\dagger P_+ \right\} \psi(x), \quad P_\pm = \frac{1}{2}(1 \pm \gamma_5), \tag{3}
$$
where the quark fields $\bar{\psi}(x), \psi(x)$ carry a (suppressed) flavour index $r = 1, \ldots, N_f$. There is, in this case, no need to include the usual term, $i\theta Q$, proportional to the topological charge $Q$ in the QCD action, since it can be traded for a phase factor of the mass matrix through an anomalous chiral transformation.

3. The chiral symmetry of the lattice theory implies that the mass matrix and the quark densities renormalize multiplicatively. Moreover, the renormalization constants of the densities may be set to the inverse of the one of the mass matrix. In the following, a massless renormalization scheme is assumed and $M, S_{rs}(x)$ and $P_{rs}(x)$ denote the renormalized mass matrix and densities.

On the lattice, the QCD partition function $Z(M)$ is a well-defined function of $M$ and so is the free energy

$$F(M) = -\ln\{Z(M)\}. \tag{4}$$

Any connected correlation function of the quark densities at zero momentum can be obtained from the free energy through repeated differentiation with respect to the real and imaginary parts of the mass matrix. Particularly useful in this context are the differential operators $\partial^S_{rs}$ and $\partial^P_{rs}$ implicitly defined by the equations

$$\partial^S_{rs}S_F = a^4 \sum_x S_{rs}(x), \quad \partial^P_{rs}S_F = a^4 \sum_x P_{rs}(x). \tag{5}$$

An example of a correlation function derived from the free energy is then

$$\partial^P_{12}\partial^S_{23}\partial^S_{31}F(M) = a^{12}\sum_{x_1,x_2,x_3}\langle P_{12}(x_1)S_{23}(x_2)S_{31}(x_3)\rangle_c \tag{6}$$

where $a$ is the lattice spacing and $\langle \ldots \rangle_c$ denotes the connected part of the lattice QCD expectation value $\langle \ldots \rangle$.

The free energy $F(M)$ is invariant under parity $M \rightarrow M^\dagger$ and charge conjugation $M \rightarrow MT$. Under infinitesimal vector and axial-vector flavour transformations of the mass matrix by an arbitrary anti-Hermitian flavour matrix $\lambda$,

$$\delta^V_\lambda M = [\lambda, M], \quad \delta^A_\lambda M = \{\lambda, M\}, \tag{7}$$

it transforms according to

$$\delta^V_\lambda F(M) = 0, \quad \delta^A_\lambda F(M) = -2\text{tr}\{\lambda\langle Q\rangle\}. \tag{8}$$
A second application of the axial transformation,

\[ \delta^A_\eta \langle Q \rangle = 2 \text{tr}\{\eta\} \langle Q^2 \rangle_c, \]  

(9)

then links the free energy to the topological susceptibility. Equations (8) and (9) follow, purely algebraically, from the definition and chiral symmetry of the lattice theory [13]. In particular, the chiral anomaly [the term proportional to \( \langle Q \rangle \) in eq. (8)] derives from the transformation behaviour of the fermion integration measure.

The lattice version of the density-chain correlation function on the right of eq. (2) is exactly equal to \( \langle Q^2 \rangle/V \) for any non-zero value of the lattice spacing [5]. If both sides of this equation are expressed through the free energy, the relation

\[ \frac{1}{6} \left\{ \delta^A_\lambda \delta^A_\eta F(M) \right\}_{M = M_m} = m_1 \ldots m_5 \{ \partial^P_{12} \partial^S_{23} \partial^S_{31} \partial^P_{45} \partial^S_{54} F(M) \}_{M = M_m} \]  

(10)

is obtained, where \( M_m = \text{diag}(m_1, \ldots, m_{N_f}) \) and

\[ \lambda = \frac{i}{2} \text{diag}(1,1,1,0,\ldots,0), \quad \eta = \frac{i}{2} \text{diag}(0,0,1,1,0,\ldots,0), \]  

(11)

are diagonal matrices, the latter acting on the first three and next two quark flavours, respectively. It may be worth mentioning in passing that eq. (10) is a consequence of the chiral symmetry properties of the free energy, i.e. of eqs. (7)-(9), but the proof of this statement is too long to be included here.

4. Correlation functions of the quark densities in general develop non-integrable short-distance singularities in the continuum limit. The free energy \( F(M) \) therefore requires additive renormalization by a counterterm \( \Delta F(M) \) before the limit can be taken. Power counting implies that the counterterm must be a polynomial of degree at most 4 in the matrix elements of \( M \) and \( M^\dagger \). Moreover, since the free energy and hence its divergent parts are invariant under the non-anomalous flavour symmetries, the counterterm may be chosen to be invariant too.

Taking these remarks into account, the counterterm must be of the form

\[ \Delta F(M) = V \left[ k_0 + \frac{k_1}{a^2} \text{tr}\{M^\dagger M\} + k_2 \text{tr}\{M^\dagger M\}^2 + k_3 \text{tr}\{(M^\dagger M)^2\} \right] \]  

(12)

with some coefficients \( k_0, \ldots, k_3 \) that depend on the gauge coupling and the renormalization scale in units of the lattice spacing. Since \( N_f \geq 5 \) is assumed, a divergent
term proportional to the real part of $\det M$ is excluded and this in turn implies that the renormalized free energy

$$\hat{F}(M) = F(M) + \Delta F(M)$$

(13)

transforms like $F(M)$ under both singlet and non-singlet flavour transformations. In particular,

$$\delta^A \hat{F}(M) = -2 \text{tr}\{\lambda\} \langle Q \rangle,$$

(14)

which shows that $\langle Q \rangle$ does not require renormalization.

Since $\Delta F(M)$ is annihilated by the axial variations $\delta^A$ as well as by any product of more than 4 derivatives with respect to the elements of the mass matrix, the unrenormalized free energy may be replaced by the renormalized one on both sides of eq. (10). The continuum limit can then be taken and, recalling eq. (2), this leads to the representation

$$\chi^{dc}_t = \frac{1}{6V} \{ \delta^A \delta^A \hat{F}(M) \}_{M=M_m}$$

(15)

of $\chi_t^{dc}$, where $\lambda$ and $\eta$ are as in eq. (11).

5. Contact with the topological charge at positive gradient-flow time is now made in the continuum theory through the small flow-time expansion

$$q(t, x) \sim \sum_{t \to 0} \sum_{k=1}^{\infty} c_k(t) \phi_k(x)$$

(16)

of the flowed topological charge density \cite{2,6,15,16}. The fields on the right of eq. (16) are renormalized local fields at flow time $t = 0$ of increasing dimension $d_k$. As $t \to 0$ and up to logarithmically varying factors, the coefficients $c_k(t)$ scale proportionally to $t^{d_k/2-2}$.

The fields $\phi_k(x)$ must be polynomials in the elements of the mass matrix $M$, the basic fields and their derivatives. They must have the same symmetry properties as the charge density, where it is understood that $M$ is treated as a “spurion”. Fields satisfying these conditions have dimension $d_k \geq 4$ and the ones of dimension 4 are

$$\phi_1(x) = q(x) + Z_{qA} \partial_\mu A^s_\mu(x),$$

(17)

$$\phi_2(x) = Z_A \partial_\mu A^s_\mu(x),$$

(18)
$q(x)$ being the bare charge density, $A^s_\mu(x)$ the bare flavour-singlet axial current, $Z_{qA}$ a (divergent) mixing coefficient and $Z_A$ the axial-current renormalization constant. The mass term

$$\sum_{r,s}\{(M^\dagger - M)_{rs}S_{rs}(x) + (M^\dagger + M)_{rs}P_{rs}(x)\}$$  \hspace{1cm} (19)$$

and the “field” $\det M^\dagger - \det M$ have the required symmetry properties too, but the latter has dimension $N_f \geq 5$ and the mass term is omitted, because it is linearly related to the fields (17),(18) through the singlet axial-current conservation equation. On the lattice, the absence of a multiplicative renormalization of the charge density in eq. (17) is implied by the chiral Ward identities \[17\], while in the case of dimensional regularization it was recently shown to derive from the special algebraic properties of the charge density \[18\].

The exact asymptotic behaviour of the coefficients $c_1(t)$ and $c_2(t)$ near $t = 0$ can be worked out in perturbation theory \[2,15\]. To this end, they are first expanded in powers of the renormalized gauge coupling $g$ and the series is then resummed using the renormalization group. The coefficients have already been computed to one-loop order \[16\], but here it suffices to know that

$$c_1(t) = 1 + O(g^2), \quad c_2(t) = O(g^4),$$  \hspace{1cm} (20)$$

and that the anomalous-dimension matrix of the fields (17),(18) is of order $g^4$. Together with the renormalization group, these properties imply

$$\lim_{t \to 0} q(t, x) = \hat{q}_{\text{RGI}}(x),$$  \hspace{1cm} (21)$$

where $\hat{q}_{\text{RGI}}(x)$ is the renormalization-group-invariant charge density (the normalization conventions are as in ref. \[18\]).

6. At this point, the equality of the gradient-flow and the density-chain expressions for the topological susceptibility can be shown in a few lines. First note that

$$\langle Q_t^2 \rangle_c = \langle Q_t Q \rangle_c$$  \hspace{1cm} (22)$$

in view of the independence of the charge $Q_t$ on the flow time $t$, the small flow-time limit (21) and the fact that $\hat{q}_{\text{RGI}}(x)$ coincides with $q(x)$ up to a term proportional to the divergence of the singlet axial current. The correlation function $\langle Q_t Q \rangle_c$ does
not require renormalization and may be represented through

\[ \langle Q_t Q \rangle_c = \frac{1}{3i} \delta^A_\lambda \langle Q_t \rangle, \]  

(23)

where \( \lambda \) is given by eq. (11).

For the same reasons (\( t \)-independence, etc.),

\[ \langle Q_t \rangle = \langle Q \rangle = -\frac{1}{2i} \delta^A_\eta \hat{F}(M), \]  

(24)

and the combination of eqs. (22)-(24) then implies

\[ \langle Q^2_t \rangle_c = \frac{1}{6} \delta^A_\lambda \delta^A_\eta \hat{F}(M). \]  

(25)

After setting \( M \) to \( M_m \) and recalling eq. (15), \( \chi^{fl}_t \) is thus seen to coincide with \( \chi^{dc}_t \).

7. If there are less than 5 flavours of sea quarks, valence quarks are included in the theory and the equivalence of the density-chain and the gradient-flow representations of the topological susceptibility can then again be proved following the lines of the previous sections. More precisely, the theory is set up with \( N_f \) fermionic and \( N_b \leq N_f \) bosonic quark fields with mass matrices \( M \) and \( \tilde{M} \), respectively, such that the effects of the first \( N_b \) fermionic quark fields are canceled if the mass matrices match. The net number of sea quarks is then \( N_f - N_b \), while \( N_b \) can be arbitrarily large and is assumed to be at least 5 in the following.

In this theory, there are separate flavour symmetries acting on the two types of quark fields and additionally a supersymmetry that mixes the bosonic with the first \( N_b \) fermionic fields. These symmetries imply that the counterterm required to cancel the singularities of the free energy \( F(M, \tilde{M}) \) must be of the form

\[
\Delta F(M, \tilde{M}) = V \left[ \frac{k_0}{a^4} + \frac{k_1}{a^2} (\text{tr}\{M^\dagger M\} - \text{tr}\{\tilde{M}^\dagger \tilde{M}\}) \right.

+ k_2 (\text{tr}\{M^\dagger M\} - \text{tr}\{\tilde{M}^\dagger \tilde{M}\})^2 + k_3 (\text{tr}\{(M^\dagger M)^2\} - \text{tr}\{(\tilde{M}^\dagger \tilde{M})^2\}) \right].
\]

(26)

Moreover, although there is now a second flavour-singlet axial current, \( \tilde{A}_\mu^a(x) \), constructed from the bosonic quark fields, the symmetries imply that there are still only
two fields of dimension 4,

\[ \phi_1(x) = q(x) + \mathcal{Z}_A \partial_\mu (A^s_\mu(x) + \tilde{A}^s_\mu(x)), \]  
\[ \phi_2(x) = \mathcal{Z}_A \partial_\mu (A^s_\mu(x) + \tilde{A}^s_\mu(x)), \]  
\[ (27) \]

which can occur in the small flow-time expansion (16).

The density-chain expression for the topological susceptibility can now be shown to coincide with the gradient-flow expression by repeating the steps taken in the case of the theory with 5 or more flavours of sea quarks. In this derivation, the bosonic quark fields play a spectator rôle and the associated mass matrix \( \tilde{M} \) can be set to the diagonal matrix with diagonal elements \( m_1, \ldots, m_{N_b} \) from the beginning.

8. Unlike the chiral anomaly, which is a robust property of the local field algebra, topological concepts are not obviously meaningful in quantum field theory, since the fluctuations of the fields integrated over in the functional integral are typically highly irregular. Along the Yang–Mills gradient flow, the high-frequency fluctuations of the gauge field in QCD are damped consistently with the renormalization group, which permits the division of field space in sectors of fixed topological charge to be given a well-defined and regularization-independent meaning [1].

The fact that the associated topological susceptibility coincides with the density-chain expression (2) shows that these sectors are related to the chiral anomaly as suggested by semi-classical studies, where the background fields are assumed to be smooth. While this has long been suspected to be the case, proving the equality of the two expressions for the susceptibility requires control over the theory at the non-perturbative level, which is, at present, only achievable through working hypotheses such as the assumption that the continuum limit of lattice QCD exists and that the small flow-time expansion (16) holds beyond perturbation theory.

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References

[1] M. Lüscher, Properties and uses of the Wilson flow in lattice QCD, JHEP 1008 (2010) 071 [Erratum: ibid. 1403 (2014) 092]
[2] M. Lüscher, P. Weisz, *Perturbative analysis of the gradient flow in non-Abelian gauge theories*, JHEP 1102 (2011) 051
[3] K. Hieda, H. Makino, H. Suzuki, *Proof of the renormalizability of the gradient flow*, Nucl. Phys. B918 (2017) 23
[4] L. Giusti, G. C. Rossi, M. Testa, *Topological susceptibility in full QCD with Ginsparg–Wilson fermions*, Phys. Lett. B587 (2004) 157
[5] M. Lüscher, *Topological effects in QCD and the problem of short distance singularities*, Phys. Lett. B593 (2004) 296
[6] M. Cè, C. Consonni, G. P. Engel, L. Giusti, *Non-Gaussianities in the topological charge distribution of the SU(3) Yang–Mills theory*, Phys. Rev. D92 (2015) 074502
[7] C. Alexandrou et al., *Topological susceptibility from twisted mass fermions using spectral projectors and the gradient flow*, Phys. Rev. D97 (2018) 074503
[8] P. H. Ginsparg, K. G. Wilson, *A remnant of chiral symmetry on the lattice*, Phys. Rev. D25 (1982) 2649
[9] D. B. Kaplan, *A method for simulating chiral fermions on the lattice*, Phys. Lett. B288 (1992) 342
[10] P. Hasenfratz, V. Laliena, F. Niedermayer, *The index theorem in QCD with a finite cutoff*, Phys. Lett. B427 (1998) 125
[11] P. Hasenfratz, *Prospects for perfect actions*, Nucl. Phys. B (Proc. Suppl.) 63 (1998) 53; *Lattice QCD without tuning, mixing and current renormalization*, Nucl. Phys. B525 (1998) 401
[12] H. Neuberger, *Exactly massless quarks on the lattice*, Phys. Lett. B417 (1998) 141; *More about exactly massless quarks on the lattice*, Phys. Lett. B427 (1998) 353
[13] M. Lüscher, *Exact chiral symmetry on the lattice and the Ginsparg–Wilson relation*, Phys. Lett. B428 (1998) 342
[14] F. Niedermayer, *Exact chiral symmetry, topological charge and related topics*, Nucl. Phys. Proc. Suppl. 73 (1999) 105
[15] M. Lüscher, *Future applications of the Yang–Mills gradient flow in lattice QCD*, PoS LATTICE2013 (2014) 016
[16] K. Hieda, H. Suzuki, *Small flow-time representation of fermion bilinear operators*, Mod. Phys. Lett. A 31 (2016) 38
[17] L. Giusti, G. C. Rossi, M. Testa, G. Veneziano, *The $U_A(1)$ problem on the lattice with Ginsparg–Wilson fermions*, Nucl. Phys. B628 (2002) 234
[18] M. Lüscher, P. Weisz, *Renormalization of the topological charge density in QCD with dimensional regularization*, Eur. Phys. J. C81 (2021) 519