

Chiral Ward identities, automatic $O(a)$ improvement and the gradient flow

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Abstract

Non-singlet chiral Ward identities for fermionic operators at positive flow-time are derived using standard techniques based on local chiral variations of the action and of local operators. The gradient flow formalism is applied to twisted mass fermions and it is shown that automatic $O(a)$ improvement for Wilson twisted mass fermions at maximal twist is a property valid also at positive flow-time. A definition of the chiral condensate that is multiplicatively renormalizable and automatically $O(a)$ improved is then derived.

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1. Introduction

The gradient flow (GF), for gauge [1] and fermion [2] fields, used in combination with a lattice regulator, can probe the non-perturbative dynamics of QCD in advantageous manners. It is defined by a differential equation that gauge and fermion fields satisfy as a function of the space–time coordinates x and of a new scale, the flow-time t . In a way the flow equations modify the short-distance behavior of local fields and can be considered as a continuous form of stout smearing [3].

Smearing has been a useful tool for lattice gauge theories since many years [4,5,3]. It was never clear though whether smeared operators had a continuum limit or not. The only exception was the discussion of the continuum limit for smeared Wilson loops in a paper by Narayanan and Neuberger [6].

The works by Lüscher and Weisz [1,7,2] give us a complete understanding of the continuum limit of observables at non-vanishing flow-time. This allows us to use the GF to define observables that otherwise would be difficult to compute with standard methods. For example

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the GF has been used to give operational definitions to the fundamental parameters of QCD as the strong coupling [1,8,9] or other quantities, as the chiral condensate [2] and the energy–momentum tensor [10,11]. The GF can also be used to define new relative ways to set the scale in lattice QCD calculations [1,12] or to define a renormalization scheme for fermionic operators [13].

To study correlation functions involving fields at positive flow-time it is, in some cases, advantageous to consider a suitable extra-dimensional local field theory where the flow-time t is the extra-dimensional coordinate and QCD is located at the $t = 0$ boundary. The theory contains the fundamental fields and appropriate Lagrange multipliers to guarantee that the fundamental fields, once the Lagrange multipliers are integrated out, satisfy the proper GF equations at positive flow-time.

In this work we derive non-singlet chiral Ward identities considering the transformation properties of the action and of local operators under a local chiral variation. We derive axial and vector Ward identities when the local variation is performed at the $t = 0$ boundary and bulk Ward identities that defines $4 + 1$ conserved axial and vector currents. To obtain the Ward identities we use two different perspectives.

The first one takes into account the dependence of the GF equations solutions on the initial conditions. A local chiral variation of the initial conditions propagates into a variation of local fields located in the bulk. Using the Lagrange multipliers it is possible to obtain a universal formula that relates the chiral variation located at the boundaries with a multilocal correlation function that depends exclusively on the type of symmetry transformation. This generates additional terms to the standard Ward identities. The same idea has been investigated in [11] in the context of space–time symmetries.

The second is to consider fermion fields at positive flow-time simply as integration variables of the extra-dimensional theory. We extend the $SU(N_f)_L \times SU(N_f)_R$ chiral symmetry transformations for the fermion fields and the corresponding Lagrange multipliers at positive flow-time. It becomes clear then that the QCD chiral Ward identities get modified by boundary terms. These boundary terms are identical to the additional terms obtained with the previous method. This second approach provides a general framework to determine Ward identities in the bulk and at the boundary of the $4 + 1$ theory that can be easily extended to any operator one is interested in. As a check we compare the chiral Ward identities with the identities obtained by Lüscher in [2] finding perfect agreement.

Chiral symmetry transformations for the $(4 + 1)$ -dimensional theory have several applications. In this work, after extending the GF formalism for twisted mass fermions, we prove automatic $O(a)$ improvement for correlators computed with Wilson twisted mass fermions at maximal twist at non-zero flow-time. As a by-product we show that the newly proposed way to determine the chiral condensate with standard Wilson fermions [2] can be easily generalized to Wilson twisted mass with the additional advantage that there is no need to determine any improvement coefficient.

2. Gradient flow

In this section, to fix the notation, we give a short introduction to the GF for gauge and fermions fields [1,2]. We consider the $SU(N)$ gauge potential, $G_\mu(x)$ and the quark and anti-quark fields $\psi(x)$ and $\bar{\psi}(x)$. The Dirac, color and flavor indices, unless specifically needed, are suppressed for simplicity.

The Yang–Mills gradient flow [1] of gauge fields as a function of the flow-time t is defined as follows

$$\partial_t B_\mu = D_{\nu,t} G_{\nu\mu}, \quad (2.1)$$

where

$$G_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu + [B_\mu, B_\nu], \quad D_{\mu,t} = \partial_\mu + [B_\mu, \cdot], \quad (2.2)$$

and the initial condition on the flow-time-dependent field $B_\mu(t, x)$ at $t = 0$ is given by the fundamental gauge field. The flow-time t has a time-squared dimension, but in the following, with a slight abuse of notation, we will refer to it as a single extra-dimension.

The flow for the quark fields considered in Ref. [2] is given by

$$\partial_t \chi_t = \Delta \chi_t, \quad \partial_t \bar{\chi}_t = \bar{\chi}_t \bar{\Delta}, \quad (2.3)$$

$$\Delta = D_{\mu,t} D_{\mu,t}, \quad D_{\mu,t} = \partial_\mu + B_\mu, \quad (2.4)$$

$$\bar{\Delta} = \bar{D}_{\mu,t} \bar{D}_{\mu,t}, \quad \bar{D}_{\mu,t} = \bar{\partial}_\mu - B_\mu, \quad (2.5)$$

which, together with the initial conditions

$$\chi_t|_{t=0} = \psi, \quad \bar{\chi}_t|_{t=0} = \bar{\psi}, \quad (2.6)$$

define the time-dependent quark and antiquark fields $\chi_t(x)$ and $\bar{\chi}_t(x)$. In the following we will indicate with $\chi_t(x)$ and $\bar{\chi}_t(x)$ the solutions of the GF equations and with $\chi(t, x)$ and $\bar{\chi}(t, x)$ generic fermion fields functions of (t, x) . We note that the GF equations for the fermion fields contain the gauge fields evolved with Eq. (2.1).

Solving the GF equations at tree-level it becomes clear the smoothing effect

$$\chi_t(x) = \int d^4y K(t; x - y) \psi(y), \quad K(t; x) = \frac{e^{-\frac{x^2}{4t}}}{(4\pi t)^2}, \quad (2.7)$$

with smearing radius of $\sqrt{8t}$.

Using the solutions of the flow equations we can construct operators located at positive flow-time and consider correlation functions between them. Correlation functions of operators located at positive flow-time can be shown to be equivalent to correlation functions defined in a local field theory in $4 + 1$ dimensions, the extra dimension being the flow-time [14,15,1,2]. The fields content of the $4 + 1$ field theory consists of the gauge and fermion fields at vanishing flow-time, at positive flow-time and the corresponding Lagrange multipliers. The Lagrange multipliers are needed to make sure that once they are integrated over the gauge and fermion fields satisfy the appropriate flow equations. The local extra-dimensional theory is a useful theoretical tool to investigate correlators involving operators at positive flow-time. For example the renormalizability of the pure-gauge gradient flow has been established [7] to all orders of perturbation theory.

In this work we consider only the fermionic sector of the theory and details about the gauge sector, the ghost sector and the gauge fixing terms can be found in Refs. [1,2]. The fermionic part of the action reads

$$S_F = S_{F,\text{QCD}} + S_{F,\text{fl}}, \quad (2.8)$$

where $S_{F,\text{QCD}}$ is the usual fermionic QCD action including the quark and gauge fields at zero flow-time

$$S_{\text{F,QCD}} = \int d^4x \bar{\psi}(x) [\gamma_\mu D_\mu + M] \psi(x), \quad (2.9)$$

where M is the mass matrix of the theory and $D_\mu = \partial_\mu + G_\mu$. The bulk action $S_{\text{F,fl}}$ of the $(4+1)$ -dimensional theory including the fields at non-zero flow-time is given by

$$S_{\text{F,fl}} = \int_0^\infty dt \int d^4x [\bar{\lambda}(t, x)(\partial_t - \Delta)\chi(t, x) + \bar{\chi}(t, x)(\overleftarrow{\partial}_t - \overleftarrow{\Delta})\lambda(t, x)], \quad (2.10)$$

where $\lambda(t, x)$ and $\bar{\lambda}(t, x)$ are the Lagrange multiplier for the fermion fields and have energy-dimension of $(4+1)/2$. The relative sign between the two terms in Eq. (2.10) is dictated by charge conjugation symmetry defined in Appendix A. Integrating out the Lagrange multipliers one identifies correlation functions of fields evolved with their flow equations to correlation functions in a local field theory in $4+1$ dimensions, the extra dimension being the flow-time.

If we consider a perturbative expansion, like for example in dimensional regularization, a gauge fixing term should be added to the action. In the following we will consider Ward identities (WIs) involving gauge invariant operators, thus all possible additional contributions coming from the gauge-fixing terms vanishes and we can safely discard them. Additionally we will always have in mind a non-perturbative definition of the theory using a lattice regulator where gauge-fixing terms are not needed.

3. Chiral symmetry

A global $SU_L(N_f) \times SU_R(N_f)$ chiral symmetry transformation

$$\begin{cases} \psi(x) \rightarrow \exp\left\{i\left(\alpha_V^a \frac{T^a}{2} + \alpha_A^a \frac{T^a}{2} \gamma_5\right)\right\} \psi(x), \\ \bar{\psi}(x) \rightarrow \bar{\psi}(x) \exp\left\{i\left(-\alpha_V^a \frac{T^a}{2} + \alpha_A^a \frac{T^a}{2} \gamma_5\right)\right\}, \end{cases} \quad (3.1)$$

leaves the massless QCD continuum action invariant. $T^a/2$ are the generators of the $SU(N_f)$ flavor group in the fundamental representation (e.g. Pauli matrices for $N_f = 2$, Gell-Mann matrices for $N_f = 3$ with $a = 1, \dots, N_f^2 - 1$) and they satisfy

$$\begin{aligned} \text{Tr}[T^a T^b] &= 2\delta^{ab}, & \left[\frac{T^a}{2}, \frac{T^b}{2}\right] &= if^{abc} \frac{T^c}{2}, \\ \left\{\frac{T^a}{2}, \frac{T^b}{2}\right\} &= id^{abc} \frac{T^c}{2} + \frac{\delta^{ab}}{2} \mathbb{1}, \end{aligned} \quad (3.2)$$

where f^{abc} are the $SU(N_f)$ structure constants, d^{abc} are symmetric coefficients. Using standard methods considering an infinitesimal local chiral transformation

$$\begin{cases} \delta\psi(x) = \left[i\alpha_V^a(x) \frac{T^a}{2} + i\alpha_A^a(x) \frac{T^a}{2} \gamma_5\right] \psi(x), \\ \delta\bar{\psi}(x) = \bar{\psi}(x) \left[-i\alpha_V^a(x) \frac{T^a}{2} + i\alpha_A^a(x) \frac{T^a}{2} \gamma_5\right], \end{cases} \quad (3.3)$$

the corresponding Noether currents, the so-called axial and vector currents, can be determined

$$A_\mu^a(x) = \bar{\psi}(x) \gamma_\mu \gamma_5 \frac{T^a}{2} \psi(x), \quad V_\mu^a(x) = \bar{\psi}(x) \gamma_\mu \frac{T^a}{2} \psi(x), \quad (3.4)$$

and the variations of the action reads

$$i \frac{\delta S_{\text{QCD}}}{\delta \alpha_A^a(x)} = \partial_\mu A_\mu^a(x) - \bar{\psi}(x) \gamma_5 \left\{ \frac{T^a}{2}, M \right\} \psi(x), \quad (3.5)$$

$$i \frac{\delta S_{\text{QCD}}}{\delta \alpha_V^a(x)} = \partial_\mu V_\mu^a(x) + \bar{\psi}(x) \left[\frac{T^a}{2}, M \right] \psi(x). \quad (3.6)$$

For a generic observable $\mathcal{O}$ the variation under the transformations (3.3) is

$$i \frac{\delta \mathcal{O}}{\delta \alpha_A^a(x)} = - \left\{ \bar{\psi}(x) \left[\gamma_5 \frac{T^a}{2} \right] \frac{\delta \mathcal{O}}{\delta \bar{\psi}(x)} - \frac{\delta \mathcal{O}}{\delta \psi(x)} \left[\gamma_5 \frac{T^a}{2} \right] \psi(x) \right\}, \quad (3.7)$$

$$i \frac{\delta \mathcal{O}}{\delta \alpha_V^a(x)} = \left\{ \bar{\psi}(x) \left[\frac{T^a}{2} \right] \frac{\delta \mathcal{O}}{\delta \bar{\psi}(x)} + \frac{\delta \mathcal{O}}{\delta \psi(x)} \left[\frac{T^a}{2} \right] \psi(x) \right\}. \quad (3.8)$$

3.1. Operators at positive flow-times

In this section we want to derive non-singlet chiral WIs when the probe operator $\mathcal{O}$ depends on quark and gauge fields solutions of the GF equations (2.1), (2.3). We derive the variations of the action and the probe operator in the classical theory. We then consider an interacting theory where a sensible regulator, as the lattice or dimensional regularization, is used. Once the local fields are properly renormalized and the regulator is removed we expect the same WIs to be valid for the renormalized fields [16].

To determine the form of the chiral WIs we need to understand how the operator $\mathcal{O}$ transforms under a local chiral transformation. A local chiral transformation of fermion fields at vanishing flow-time modifies the initial conditions of the flow-equations. Consequently the fermion fields solutions of the flow equations at positive flow-time are altered. In other words the transformation properties under chiral symmetry of the fermion fields at vanishing flow-time are propagated to the fermion fields at non-vanishing flow-time.

These variations can be determined considering the functional dependence of the fermion fields at positive flow-time from the initial conditions of the flow equations, i.e. evaluating the following expression

$$i \frac{\delta \mathcal{O}}{\delta \alpha_A^a(x)} = - \int_0^\infty dt \int d^4z \left\{ \left[\bar{\psi}(x) \gamma_5 \frac{T^a}{2} \right] \bar{J}(t, z; 0, x) \frac{\delta \mathcal{O}}{\delta \bar{\chi}_t(z)} + \left[\gamma_5 \frac{T^a}{2} \psi(x) \right] J(t, z; 0, x) \frac{\delta \mathcal{O}}{\delta \chi_t(z)} \right\}, \quad (3.9)$$

where the Jacobians are defined as

$$J(t, z; s, x) = \theta(t-s) \frac{\delta \chi_t(z)}{\delta \chi_s(x)}, \quad \bar{J}(t, z; s, x) = \theta(t-s) \frac{\delta \bar{\chi}_t(z)}{\delta \bar{\chi}_s(x)}. \quad (3.10)$$

Eq. (3.9) is a non-local expression due to the presence of the Jacobian matrices J and $\bar{J}$, thus it would be rather difficult to study its divergences and renormalization properties. This problem can be solved if the operator $\mathcal{O}$ does not depend on the Lagrange multipliers λ and $\bar{\lambda}$. In fact in this specific case it is possible to evaluate the expression on the r.h.s. of Eq. (3.9) obtaining

$$\left\langle i \left[\frac{\delta \mathcal{O}}{\delta \alpha_A^a(x)} \right]_R \right\rangle = - \langle \mathcal{O}_R \tilde{P}_R^a(0, x) \rangle, \quad (3.11)$$

where

$$\tilde{P}^a(t, x) = \bar{\lambda}(t, x) \frac{T^a}{2} \gamma_5 \chi(t, x) + \bar{\chi}(t, x) \frac{T^a}{2} \gamma_5 \lambda(t, x), \quad (3.12)$$

and

$$\tilde{P}_R^a = Z_{\tilde{P}} \tilde{P}^a. \quad (3.13)$$

The renormalization of $Z_{\tilde{P}}$, discussed in Ref. [2], is multiplicative and it turns out to be equal to one even if the interacting theory is regularized with Wilson fermions. If the operator $\mathcal{O}$ contains only fermion and gauge fields at positive flow-times and does not contain Lagrange multipliers it renormalizes multiplicatively [2] depending on the total number n of fermion and anti-fermion fields, i.e.

$$\mathcal{O}_R = [Z_\chi]^{n/2} \mathcal{O}, \quad (3.14)$$

where Z_χ is the normalization factor for the fermion fields and Lagrange multipliers at positive flow-time $\chi_R = Z_\chi^{1/2} \chi$, $\lambda_R = Z_\chi^{-1/2} \lambda$.

Eq. (3.11) is a specific case of a more general result (see Appendix B for the derivation) that we can formally write as

$$\begin{aligned} & \frac{1}{\mathcal{Z}_{\chi, \lambda}} \int \mathcal{D}[\chi, \bar{\chi}] \mathcal{D}[\lambda, \bar{\lambda}] \mathcal{O}[\bar{\lambda}(s, x) \Gamma^a(s, x) + \bar{\Gamma}^a(s, x) \lambda(s, x)] \exp\{-S_{F, \Pi}\} \\ &= \int_s^\infty dt \int d^4 z \left[\bar{\Gamma}^a(s, x) \bar{J}(t, z; s, x) \frac{\delta \mathcal{O}}{\delta \bar{\chi}(t, z)} \right. \\ & \quad \left. + \Gamma^a(s, x) J(t, z; s, x) \frac{\delta \mathcal{O}}{\delta \chi(t, z)} \right]_0, \end{aligned} \quad (3.15)$$

where

$$\mathcal{Z}_{\chi, \lambda} = \int \mathcal{D}[\chi, \bar{\chi}] \mathcal{D}[\lambda, \bar{\lambda}] \exp\{-S_{F, \Pi}\}, \quad (3.16)$$

and the index 0 indicates that the r.h.s. of Eq. (3.15) has to be evaluated with fields χ and $\bar{\chi}$ solutions of the GF equations.

Eq. (3.15) is useful because it relates the symmetry transformation of $\mathcal{O}$, induced by the boundary conditions, to a multi-local correlation function whose form is solely dictated by the type of transformation, here parametrized by the functions Γ and $\bar{\Gamma}$. Additionally the equation is valid if $\mathcal{O}$, Γ^a and $\bar{\Gamma}^a$ do not depend on the Lagrange multipliers λ and $\bar{\lambda}$.

We are now in the position to derive the chiral WIs using standard techniques obtaining

$$\langle [\partial_\mu A_{\mu, R}^a(x) - P_R^{[a, MR]}(x) + \tilde{P}_R^a(0, x)] \mathcal{O}_R \rangle = 0, \quad (3.17)$$

$$\langle [\partial_\mu V_{\mu, R}^a(x) + S_R^{[a, MR]}(x) + \bar{S}_R^a(0, x)] \mathcal{O}_R \rangle = 0, \quad (3.18)$$

where

$$\bar{S}_R^a = Z_{\bar{S}} \bar{S}^a, \quad (3.19)$$

and

$$\bar{S}^a(t, x) = \bar{\lambda}(t, x) \frac{T^a}{2} \chi(t, x) - \bar{\chi}(t, x) \frac{T^a}{2} \lambda(t, x). \quad (3.20)$$

The renormalization of $\tilde{S}^a$ following the same argumentation used for $\tilde{P}^a$ is also multiplicative. For a generic mass matrix the scalar and pseudoscalar densities read

$$P_R^{[a, M_R]}(x) = Z_P \bar{\psi}(x) \gamma_5 \left\{ \frac{T^a}{2}, M_R \right\} \psi(x), \quad (3.21)$$

and

$$S_R^{[a, M_R]}(x) = Z_S \bar{\psi}(x) \left[\frac{T^a}{2}, M_R \right] \psi(x). \quad (3.22)$$

Eq. (3.17) was already derived in Ref. [2] using the defining equations for the fermion propagators and Wick contractions. It is interesting to see that the same relation can be obtained using standard symmetry methods. This derivation also elucidates the origin of the additional term proportional to $\tilde{P}^a$, i.e. it is the variation of the probe operator at positive flow-time resulting from the chiral transformation of the initial conditions of the flow equations.

Eq. (3.18) is new and is the vector WI with an external probe located at positive flow-time. In this case the variation of the external operator can be worked out using the general formula (3.15) obtaining that it is proportional to $\tilde{S}^a$.

4. Chiral symmetry at positive flow-time

A different way to derive chiral WIs at positive flow-time is to extend the chiral symmetry transformations (3.1) to the $(4 + 1)$ -dimensional theory. This extension is more general and it allows us to find the corresponding $(4 + 1)$ -dimensional Noether currents and the extension of the WIs for positive flow-time.

The chiral symmetry transformation of the fermion fields at vanishing flow-time are the standard ones for a Dirac field. The boundary conditions (2.6) extend in a natural way the $SU_L(N_f) \times SU_R(N_f)$ chiral symmetry transformations to the fermion fields and non-zero flow-time, i.e.

$$\begin{cases} \chi(t, x) \rightarrow \exp \left\{ i \left(\alpha_V^a \frac{T^a}{2} + \alpha_A^a \frac{T^a}{2} \gamma_5 \right) \right\} \chi(t, x), \\ \bar{\chi}(t, x) \rightarrow \bar{\chi}(t, x) \exp \left\{ i \left(-\alpha_V^a \frac{T^a}{2} + \alpha_A^a \frac{T^a}{2} \gamma_5 \right) \right\}. \end{cases} \quad (4.1)$$

Since the flow equations (2.3) together with the initial conditions (2.6) are invariant under the chiral transformations (3.1), the time-dependent fields transform in the same way under chiral transformations as the fields at zero flow-time. For example the scalar and pseudoscalar densities

$$S^a(t, x) = \bar{\chi}(t, x) \frac{T^a}{2} \chi(t, x), \quad P^b(t, x) = \bar{\chi}(t, x) \gamma_5 \frac{T^a}{2} \chi(t, x), \quad (4.2)$$

transform in the same way as the corresponding composite fields at vanishing flow-time [17].

We want to ask the question how the Lagrange multiplier fields λ and $\bar{\lambda}$ transform under chiral symmetry. The invariance of the flow equation for fermions can be seen as a consequence of the invariance under chiral transformation of the bulk action $S_{F,fl}$ (2.10). This implies that the chiral transformations are

$$\begin{cases} \lambda(t, x) \rightarrow \exp \left\{ i \left(\alpha_V^a \frac{T^a}{2} - \alpha_A^a \frac{T^a}{2} \gamma_5 \right) \right\} \lambda(t, x), \\ \bar{\lambda}(t, x) \rightarrow \bar{\lambda}(t, x) \exp \left\{ i \left(-\alpha_V^a \frac{T^a}{2} - \alpha_A^a \frac{T^a}{2} \gamma_5 \right) \right\}. \end{cases} \quad (4.3)$$

We note the opposite sign for the axial transformation coefficient with respect to the standard transformation. Another way to understand that these are the correct chiral transformations of the Lagrange multipliers is to consider the bulk action $S_{F,\Pi}$ and note that the Lagrange multipliers λ and $\bar{\lambda}$ are equivalent to the differential operators

$$\bar{\lambda} \rightarrow \frac{\delta}{\delta \bar{\mathcal{F}}}, \quad \lambda \rightarrow \frac{\delta}{\delta \mathcal{F}}, \quad (4.4)$$

where

$$\mathcal{F}(t, x) = [\partial_t - \Delta]\chi(t, x), \quad \bar{\mathcal{F}}(t, x) = \bar{\chi}(t, x)[\bar{\partial}_t - \bar{\Delta}]. \quad (4.5)$$

We use the chiral transformations for the fermions fields (4.1) and for the Lagrange multipliers (4.3) to derive chiral WIs. Using standard techniques we consider an infinitesimal local $SU(N_f) \times SU(N_f)$ chiral transformations of the fermionic fields

$$\begin{cases} \delta\chi(t, x) = \left[i\alpha_V^a(t, x)\frac{T^a}{2} + i\alpha_A^a(t, x)\frac{T^a}{2}\gamma_5 \right] \chi(t, x), \\ \delta\bar{\chi}(t, x) = \bar{\chi}(t, x) \left[-i\alpha_V^a(t, x)\frac{T^a}{2} + i\alpha_A^a(t, x)\frac{T^a}{2}\gamma_5 \right], \\ \delta\lambda(t, x) = \left[i\alpha_V^a(t, x)\frac{T^a}{2} - i\alpha_A^a(t, x)\frac{T^a}{2}\gamma_5 \right] \lambda(t, x), \\ \delta\bar{\lambda}(t, x) = \bar{\lambda}(t, x) \left[-i\alpha_V^a(t, x)\frac{T^a}{2} - i\alpha_A^a(t, x)\frac{T^a}{2}\gamma_5 \right]. \end{cases} \quad (4.6)$$

It is interesting to note that the densities $\tilde{P}^a$ and $\bar{S}^a$ form a multiplet as can be seen performing an infinitesimal axial and vector rotation

$$\delta_A \tilde{P}^b = f^{abc} \alpha_A^a \bar{S}^c, \quad \delta_A \bar{S}^b = f^{abc} \alpha_A^a \tilde{P}^c, \quad (4.7)$$

$$\delta_V \tilde{P}^b = f^{abc} \alpha_A^a \tilde{P}^c, \quad \delta_V \bar{S}^b = f^{abc} \alpha_A^a \bar{S}^c. \quad (4.8)$$

To take into account properly boundary effects we discretize the flow-time direction with spacing ϵ and we treat separately the cases $t = 0$ and $t > 0$. Discretizing the flow-time direction the bulk action reads

$$S_{F,\Pi} = \epsilon \sum_{t=0}^{T-\epsilon} \int d^4x \left[\bar{\lambda}(t, x)(\partial_t - \Delta)\chi(t, x) + \bar{\chi}(t, x)(\bar{\partial}_t - \bar{\Delta})\lambda(t, x) \right], \quad (4.9)$$

where

$$\partial_t \chi(t, x) = \frac{1}{\epsilon} [\chi(t + \epsilon, x) - \chi(t, x)], \quad (4.10)$$

$$\bar{\chi}(t, x) \bar{\partial}_t = \frac{1}{\epsilon} [\bar{\chi}(t + \epsilon, x) - \bar{\chi}(t, x)]. \quad (4.11)$$

The Δ operator is the lattice Laplacian

$$\Delta = \nabla_{\mu,t} \nabla_{\mu,t}^*, \quad \bar{\Delta} = \bar{\nabla}_{\mu,t} \bar{\nabla}_{\mu,t}^*, \quad (4.12)$$

where ∇_μ and ∇_μ^* are the gauge-covariant forward and backward difference operators in presence of the flow-time dependent gauge field.

Computing the local chiral variation of the action at $t = 0$ we obtain the so-called PCAC relation

$$\partial_\mu A_\mu^a(x) - P^{(a,M)}(x) + \tilde{P}^a(0, x) = 0. \quad (4.13)$$

Once again we find an additional term with respect to the standard PCAC. In the approach we are following in this section the additional term is the result of the chiral variation of the boundary terms.

We consider now a generic operator

$$\mathcal{O} = \phi_1(t_1, x_1) \cdots \phi_n(t_n, x_n), \quad (4.14)$$

where $\phi_1, \dots, \phi_n$ can be fermion or gauge fields. The WIs in the interacting theory, valid for the renormalized fields once the regulator has been removed, is identical to Eq. (3.17). Following the line of reasoning of the previous section one might wonder why we have not considered a variation of the operator $\mathcal{O}$. The reason exemplifies the differences between the two methods. In this second approach the fermion fields at positive flow-time are in general *not* solutions of the GF equations but only integration variables. As such there is no complicated dependence of these fermion fields from other fermion fields located at smaller flow-time. In the previous section the fermion fields were solutions of the GF equations, i.e. the integration over the Lagrange multipliers was already performed, thus the non-local dependence on the initial conditions. The generalization of the chiral symmetry transformations for the $(4 + 1)$ -dimensional theory gives us another tool to obtain Eq. (3.17).

Using the transformations in (4.6) we can derive bulk chiral WIs. If we perform a local axial variation at a flow-time $s > 0$ and we assume that $s < t_i$ for all the t_i arguments of $\mathcal{O}$ the axial WI after $\epsilon \rightarrow 0$ is

$$\langle [\partial_s \tilde{P}^a(s, x) + \partial_\mu \mathcal{A}_\mu^a(s, x)] \mathcal{O}_R(\{t_0\}) \rangle = 0, \quad s > 0, s < \{t_0\} \quad (4.15)$$

where we have denoted generically with $\{t_0\} = \{t_1, \dots, t_N\}$ the flow-time dependence of the operator $\mathcal{O}$. The current $\mathcal{A}_\mu^a$ is

$$\begin{aligned} \mathcal{A}_\mu^a(s, x) = & \bar{\lambda}(s, x) \frac{T^a}{2} \gamma_5 (\tilde{D}_{\mu,t} - D_{\mu,t}) \chi(s, x) \\ & - \bar{\chi}(s, x) \frac{T^a}{2} \gamma_5 (\tilde{D}_{\mu,t} - D_{\mu,t}) \lambda(s, x). \end{aligned} \quad (4.16)$$

Even if we use Wilson fermions as a lattice regulator at the boundary, the chiral symmetry of the bulk action implies that the WI (4.15) is an exact relation in the bare theory. Since we expect the same WI to be valid after renormalizing the fields and removing the regulator we can conclude that the normalization factors of $\tilde{P}^a(s, x)$ and $\mathcal{A}_\mu^a(s, x)$ are equal to one for all positive flow-times and the regulator can be safely removed. We recall that operators located at positive flow-time are renormalized with their field content and because $Z_\chi = Z_\lambda^{-1}$ the WI (4.15) for $s > 0$ is consistent with this result.

Introducing a $4 + 1$ axial current $\mathcal{A}_M$ with $M = 0, \dots, 4$ where 0 denotes the flow-time direction

$$\mathcal{A}_M^a = (\tilde{P}^a, \mathcal{A}_\mu^a), \quad (4.17)$$

we can rewrite the WI for $s > 0$ in a suggestive way

$$\langle \partial_M \mathcal{A}_M^a(s, x) \mathcal{O}_R(\{t_0\}) \rangle = 0, \quad (4.18)$$

where

$$\partial_M = (\partial_t, \partial_\mu). \quad (4.19)$$

We note a dimensional mismatch between the different components of the $(4 + 1)$ -dimensional axial current. This is a direct consequence of the different dimensionality between the Lagrange multipliers and the fermion fields that is related to the different dimensionality between the flow-time and any space–time dimension.

Integration of Eq. (4.15) over the 4-dimensional space–time leads to

$$\int d^4x \langle \partial_s \tilde{P}^a(s, x) \mathcal{O}_R(\{t_0\}) \rangle = 0. \quad (4.20)$$

This result can also be obtained using the GF equations and observing that

$$\int d^4x K(t, y; s, x) K(s, x; 0, v) = K(t, y; 0, v), \quad (4.21)$$

with $t > s > 0$. Eq. (4.20) is interesting because if we consider the short flow-time expansion

$$\tilde{P}^a(s, x) = c_{\tilde{P}}(s) \tilde{P}^a(0, x) + \mathcal{O}(s), \quad (4.22)$$

Eq. (4.20), satisfied order by order in s , immediately implies that $c_{\tilde{P}}$ is a constant and because of the renormalization group equations applied to Eq. (4.22) also independent of the coupling. A tree-level calculation thus shows that $c_{\tilde{P}}(s) = 1$.

We integrate now the WI along the flow-time direction from ϵ and t with $0 < \epsilon < t < t_i$ and we obtain

$$\langle [A_0^a(\epsilon, x) - A_0^a(t, x)] \mathcal{O}_R(\{t_0\}) \rangle = \left\langle \left[\partial_\mu \int_\epsilon^t ds A_\mu^a(s, x) \right] \mathcal{O}_R(\{t_0\}) \right\rangle. \quad (4.23)$$

To perform the limit $\epsilon \rightarrow 0$ we need to make sure that the integral in the r.h.s. has, at most, integrable singularities. One needs to classify all the operators of dimension 5 or less that can mix with $\mathcal{A}_\mu$. The first thing we notice is that the operators appearing in the short flow-time expansion of $\mathcal{A}_\mu^a$ should contain at least one Lagrange multiplier. This because otherwise any two-point function between such operators and $\mathcal{A}_\mu^a$ would vanish. This implies that there can be operators of dimension 4 or 5, but chiral symmetry, extended to the Lagrange multipliers, charge conjugation and $O(4)$ symmetry exclude them. We are left with at most a logarithmic divergence when $s \rightarrow 0$ and this divergence is integrable.

Using Eq. (3.17) we can then write

$$-\langle \tilde{P}^a(t, x) \mathcal{O}_R(\{t_0\}) \rangle = \langle [\partial_\mu \bar{A}_{\mu,R}^a(t, x) - P_R^{[a,M]}(x)] \mathcal{O}_R(\{t_0\}) \rangle, \quad (4.24)$$

where

$$\bar{A}_{\mu,R}^a(t, x) = Z_A A_\mu^a(x) + \int_0^t ds A_\mu(s, x). \quad (4.25)$$

We can interpret Eq. (4.24) as a generalization of the axial WI at positive flow-time, where the l.h.s. of Eq. (4.24), following the general result of Eq. (3.15), is the variation of the operator $\mathcal{O}$ induced by a chiral transformation performed on the quark fields at a flow-time $t < t_i$.

We show now with an example the usefulness of this approach deriving the identity obtained by Lüscher that allows to relate the chiral condensate to pseudoscalar correlation functions (cf. with Eq. (4.9) of Ref. [2]). We consider the WI in Eq. (4.18) with an operator $\mathcal{O}$ function of fermion fields localized at flow-time t . We do not assume any ordering on the flow-times thus we need to add a contact term to the WI when $t = s$ stemming from the local variation of the operator

$$\langle [\partial_s \tilde{P}^a(s, x) + \partial_\mu \mathcal{A}_\mu^a(s, x)] \mathcal{O}_R(t, y) \rangle = \left\langle i \left[\frac{\delta \mathcal{O}(t, y)}{\delta \alpha_A^a(s, x)} \right]_R \right\rangle. \quad (4.26)$$

The r.h.s. can be computed in a standard manner if we consider $\mathcal{O}(t, y) = P^b(t, y)$

$$\langle [\partial_s \tilde{P}^a(s, x) + \partial_\mu \mathcal{A}_\mu^a(s, x)] P_R^b(t, y) \rangle = -\langle S_R^{[a,b]}(s, y) \rangle \delta(t - s) \delta(x - y), \quad (4.27)$$

where

$$S^{[a,b]}(s, y) = \bar{\chi}(s, y) \left\{ \frac{T^a}{2}, \frac{T^b}{2} \right\} \chi(s, y). \quad (4.28)$$

We recall that $P^a(t, y)$ and $S^a(t, y)$ renormalize multiplicatively with Z_χ [2]. Integrating this WI over the whole 4-dimensional space–time volume we obtain

$$\int d^4x \langle \partial_s \tilde{P}^a(s, x) P_R^b(t, y) \rangle = -\langle S_R^{[a,b]}(s, y) \rangle \delta(t - s). \quad (4.29)$$

Having included the contact term we can now integrate in the flow-time in the range $\epsilon < s < T$ with $T > t$ and perform the limit $\epsilon \rightarrow 0$

$$\lim_{\epsilon \rightarrow 0} \int d^4x \int_{\epsilon}^T ds \langle \partial_s \tilde{P}^a(s, x) P_R^b(t, y) \rangle = -\lim_{\epsilon \rightarrow 0} \int_{\epsilon}^T ds \langle S_R^{[a,b]}(s, y) \rangle \delta(t - s). \quad (4.30)$$

The boundary term at T does not contribute because propagators $\overline{\lambda(T, x)} \bar{\chi}(t, x)$ and $\overline{\chi(t, x)} \bar{\lambda}(T, x)$ vanish for $T > t$ [2]. We thus obtain

$$\int d^4x \langle \tilde{P}^a(0, x) P_R^b(t, y) \rangle = \langle S_R^{[a,b]}(t, y) \rangle. \quad (4.31)$$

This is exactly the relation obtained in Ref. [2], that allows the determination of the chiral condensate (cf. Eq. 4.15 of Ref. [2]). This example shows that it is possible to use standard techniques based on chiral symmetry transformations to derive WIs involving fields at the boundary and solutions of the GF for positive flow-time.

We remark that in the derivation of Eq. (4.31) it is not necessary to send $\epsilon \rightarrow 0$. If we integrate over the flow-time between s_0 and T with $s_0 < t < T$ we obtain

$$\int d^4x \langle \tilde{P}^a(s_0, x) P_R^b(t, y) \rangle = \langle S_R^{[a,b]}(t, y) \rangle. \quad (4.32)$$

This result is independent of s_0 as far as $0 < s_0 < t$ as can be seen from Eq. (4.20). It is only to make contact with the physics of pions that it is necessary to place $\tilde{P}^a$ at the boundaries.

4.1. Vector ward identities

Using the procedure outlined in the previous section we can derive also the so-called PCVC relation at the boundary $t = 0$ and the corresponding relation in the bulk

$$\begin{cases} \partial_\mu V_\mu^a(x) + \bar{\psi}(x) \left[\frac{T^a}{2}, M \right] \psi(x) + \bar{S}^a(0, x) = 0, & t = 0, \\ \partial_t \bar{S}^a(t, x) + \partial_\mu \mathcal{V}_\mu^a(t, x) = 0, & t > 0, \end{cases} \quad (4.33)$$

where

$$\bar{S}^a(t, x) = \bar{\lambda}(t, x) \frac{T^a}{2} \chi(t, x) - \bar{\chi}(t, x) \frac{T^a}{2} \lambda(t, x), \quad (4.34)$$

and

$$\mathcal{V}_\mu^a(t, x) = \bar{\lambda}(t, x) \frac{T^a}{2} (\tilde{D}_{\mu,t} - D_{\mu,t}) \chi(t, x) + \bar{\chi}(t, x) (\tilde{D}_{\mu,t} - D_{\mu,t}) \frac{T^a}{2} \lambda(t, x). \quad (4.35)$$

As for the axial case we can rewrite the second relation in (4.33) for $t > 0$ introducing a 4 + 1 vector current $\mathcal{V}_M$ with $M = 0, \dots, 4$ where the 0 index refers to the flow-time direction

$$\mathcal{V}_M^a = (\bar{S}^a(t, x), \mathcal{V}_\mu^a(t, x)). \quad (4.36)$$

For $t > 0$ the vector current $\mathcal{V}_M^a$ is conserved

$$\partial_M \mathcal{V}_M^a = 0. \quad (4.37)$$

Using as a probe $\mathcal{O}(\{t_0\})$, the VWI with $t_0 > s$ reads

$$\langle [\partial_t \mathcal{V}_0^a(s, x) + \partial_\mu \mathcal{V}_\mu^a(s, x)] \mathcal{O}_R(\{t_0\}) \rangle = 0, \quad (4.38)$$

and the generalization of the standard VWI is

$$-\langle \bar{S}^a(t, x) \mathcal{O}(t_0, y) \rangle = \langle \partial_\mu \bar{V}_\mu^a(t, x) \mathcal{O}(\{t_0\}) \rangle, \quad (4.39)$$

where

$$\bar{V}_\mu^a(t, x) = Z_V V_\mu^a(x) + \int_0^t ds \mathcal{V}_\mu(s, x). \quad (4.40)$$

5. Twisted mass QCD

In this section we consider the GF with twisted mass fermions [18]. For simplicity we consider a flavor doublet of mass degenerate twisted mass fermions. The extension to non-degenerate twisted mass fermions [19] does not pose any additional complication. For reviews about twisted mass fermions see Refs. [20–22]. In the twisted basis the continuum twisted mass action

$$S_{\text{F,tmQCD}} = \int d^4x \bar{\psi}(x) [\gamma_\mu D_\mu + m + i\mu_q \gamma_5 \tau^3] \psi(x), \quad (5.1)$$

is obtained by a chiral rotation of a twist angle $\omega = \text{atan}(\mu_q/m)$

$$\begin{cases} \psi(x) \rightarrow \exp\left\{i\left(\omega\frac{\tau^3}{2}\gamma_5\right)\right\}\psi(x), \\ \bar{\psi}(x) \rightarrow \psi(x)\exp\left\{i\left(\omega\frac{\tau^3}{2}\gamma_5\right)\right\}, \end{cases} \quad (5.2)$$

of the continuum QCD action. To obtain the fermionic part of the action for the (4 + 1)-dimensional theory we perform the same twist rotation on the fermion fields at positive flow-time

$$\begin{cases} \chi(t, x) \rightarrow \exp\left\{i\left(\omega\frac{\tau^3}{2}\gamma_5\right)\right\}\chi(t, x), \\ \bar{\chi}(t, x) \rightarrow \bar{\chi}(t, x)\exp\left\{i\left(\omega\frac{\tau^3}{2}\gamma_5\right)\right\}. \end{cases} \quad (5.3)$$

The Lagrange multipliers are also a flavor doublet and the twist rotation is obtained using the chiral symmetry transformations defined in Eqs. (3.1), (4.3)

$$\begin{cases} \lambda(t, x) \rightarrow \exp\left\{i\left(-\omega\frac{\tau^3}{2}\gamma_5\right)\right\}\lambda(t, x), \\ \bar{\lambda}(t, x) \rightarrow \bar{\lambda}(t, x)\exp\left\{i\left(-\omega\frac{\tau^3}{2}\gamma_5\right)\right\}. \end{cases} \quad (5.4)$$

The exact chiral symmetry of the bulk term in the 4 + 1 theory implies that this term of the action stays invariant under a twist rotation, i.e. the total twisted mass action is

$$S_F = S_{F, \text{tmQCD}} + S_{F, \text{fl}}, \quad (5.5)$$

where $S_{F, \text{fl}}$ is given by Eq. (2.10). This is not surprising because the GF equations (2.3) and the initial conditions (2.6) are invariant under a twist rotation.

The twist rotations in Eqs. (5.3), (5.4) define the operators at positive flow-time in the twisted basis. Fermions bilinears formed only by fermion fields or only Lagrange multipliers transform in a standard manner. Bilinears made of fermion and Lagrange multiplier fields twist in a different way and, as an example, we show how the twist rotation applies to $\tilde{P}^a$ and $\bar{S}^a$

$$\begin{cases} \tilde{P}^a \rightarrow \cos\omega\tilde{P}^a + \sin\omega\bar{S}^a, & a = 1, 2, \\ \tilde{P}^a \rightarrow \tilde{P}^a, & a = 0, 3, \end{cases} \quad (5.6)$$

$$\begin{cases} \bar{S}^a \rightarrow \cos\omega\bar{S}^a + \sin\omega\tilde{P}^a, & a = 1, 2, \\ \bar{S}^a \rightarrow \bar{S}^a, & a = 0, 3. \end{cases} \quad (5.7)$$

Using the action in Eq. (5.5) and the chiral transformations (4.1), (4.3) we can derive the PCAC and PCVC relations

$$\begin{cases} \partial_\mu A_\mu^a(x) - 2mP^a(x) - i\mu_q\delta^{a3}S^0(x) + \tilde{P}^a(0, x) = 0, & t = 0, \\ \partial_t\tilde{P}^a(t, x) + \partial_\mu\mathcal{A}_\mu^a(t, x) = 0, & t > 0, \end{cases} \quad (5.8)$$

and

$$\begin{cases} \partial_\mu V_\mu^a(x) + 2\mu_q\epsilon^{3ab}P^b(x) + \bar{S}^a(0, x) = 0, & t = 0, \\ \partial_t\bar{S}^a(t, x) + \partial_\mu\mathcal{V}_\mu^a(t, x) = 0, & t > 0. \end{cases} \quad (5.9)$$

The equivalence between QCD and tmQCD in the interacting theory has been proven in [18] using as a regulator overlap fermions. We note that the exact chiral symmetry of the bulk action

does not add any complication and the result of [18] is valid for correlation functions involving local operators also at positive flow-time.

6. Wilson twisted mass fermions

The GF equations can be applied to a fermion field independently on the fermionic lattice action of choice. Here we choose to study the interplay between the GF and Wilson twisted mass (Wtm) fermions. In particular we want to analyze the $O(a)$ cutoff effects of this formulation for operators defined at positive flow-time and we want to see if it is possible to extend the property of automatic $O(a)$ improvement.

Since we will only be concerned with $O(a)$ effects of the $(4 + 1)$ -dimensional theory we do not need to specify the exact form of the gauge action. The form of the unimproved fermionic lattice action at the boundary $t = 0$ is

$$S_{\text{Wtm}}[\psi, \bar{\psi}, U] = a^4 \sum_x \bar{\psi}(x) [D_W + m_0 + i\mu_0 \gamma_5 \tau^3] \psi(x), \quad (6.1)$$

where D_W is the usual Wilson massless operator

$$D_W = \frac{1}{2} [\gamma_\mu (\nabla_\mu + \nabla_\mu^*) - a \nabla_\mu^* \nabla_\mu]. \quad (6.2)$$

The bulk action is the one defined in (4.9) and m_0, μ_0 are the bare untwisted and twisted quark mass.

The long distance properties of Wtm close to the continuum limit may be described in terms of a local effective theory with action

$$S_{\text{eff}} = S_0 + aS_1 + a^2S_2 + \dots \quad (6.3)$$

where the leading term, S_0 , is the action of the target continuum theory (5.5) plus the gauge action with properly renormalized parameters. The higher order terms are linear combination of higher-dimensional operators. For example

$$S_1 = \int_0^\infty dt \int d^4x \sum_i c_i (g_0^2) \mathcal{O}_{R,i}(t, x), \quad (6.4)$$

where $\mathcal{O}_i(t, x)$ respect the symmetries of the lattice action. We omit for simplicity the dependence on the renormalization scale.

A correlation function of products of a multiplicatively renormalizable lattice fields, here denoted by $\phi_R = Z_\phi \phi$, at separated points (t_i, x_i)

$$G(t_1, x_1; \dots; t_n, x_n) = \langle \phi_R(t_1, x_1) \cdots \phi_R(t_n, x_n) \rangle \equiv \langle \Phi_R \rangle \quad (6.5)$$

takes the form

$$\langle \Phi_R \rangle = \langle \Phi_0 \rangle_0 - a \langle \Phi_0 S_1 \rangle_0 + a \langle \Phi_1 \rangle_0 + O(a^2), \quad (6.6)$$

where

$$\langle \Phi_0 \rangle_0 \equiv \langle \phi_0(t_1, x_1) \cdots \phi_0(t_n, x_n) \rangle_0, \quad (6.7)$$

$$\langle \Phi_1 \rangle_0 \equiv \sum_{k=1}^n \langle \phi_0(t_1, x_1) \cdots \phi_1(t_k, x_k) \cdots \phi_0(t_n, x_n) \rangle_0, \quad (6.8)$$

and ϕ_0, ϕ_1 are renormalized continuum fields. ϕ_1 is a linear combination of local operators of dimension $d_\phi + 1$ that depends on the specific operator ϕ and are classified according to the lattice symmetries transformation properties of ϕ . The expectation values on the right hand side of Eq. (6.6) are to be taken in the continuum theory with action S_0 .

In the massless limit Wilson and Wtm fermions have the same lattice action thus the higher-dimensional operators in the Symanzik effective action are the same. Using the equations of motion for the quark fields in the chiral limit a possible list of $O(a)$ terms is [23,2]

$$\mathcal{O}_1 = i\bar{\psi}(x)\sigma_{\mu\nu}F_{\mu\nu}\psi(x), \quad \mathcal{O}_2 = \bar{\lambda}(0, x)\lambda(0, x). \quad (6.9)$$

It is important to notice that there are no t -dependent terms in the effective action. The additional operator $\mathcal{O}_2$ is a boundary term. From the point of view of the chiral symmetry transformations (4.1), (4.3) the absence of $O(a)$ terms for $t > 0$ is a consequence of the chiral invariance of the bulk action.

Additional terms in the effective theory at non-zero quark mass for Wtm fermions have been classified in [23,24]. The gradient flow adds the operators $\mathcal{O}_7$ and $\mathcal{O}_8$ to the list

$$\begin{aligned} \mathcal{O}_3 &= m \operatorname{tr}\{F_{\mu\nu}(x)F_{\mu\nu}(x)\}, & \mathcal{O}_4 &= m\bar{\psi}(x)\psi(x), & \mathcal{O}_5 &= m\mu_q i\bar{\psi}(x)\gamma_5\tau^3\psi(x), \\ \mathcal{O}_6 &= \mu_q^2\bar{\psi}(x)\psi(x), & \mathcal{O}_7 &= m(\bar{\lambda}(0, x)\psi(x) + \bar{\psi}(x)\lambda(0, x)), \\ \mathcal{O}_8 &= i\mu_q(\bar{\lambda}(0, x)\gamma_5\tau^3\psi(x) + \bar{\psi}(x)\gamma_5\tau^3\lambda(0, x)). \end{aligned} \quad (6.10)$$

The operator $\mathcal{O}_7$ is already given in Ref. [2]. The operator $\mathcal{O}_8$ is new and is the one needed to remove $O(a\mu_q)$ effects to the fermion fields and Lagrange multipliers.

6.1. Automatic $O(a)$ improvement

Automatic $O(a)$ improvement [25] is the property of Wtm that physical correlation functions with a finite continuum limit made of multiplicatively renormalizable fields are free from $O(a)$ effects, when the lattice parameters are tuned to obtain in the continuum limit that the renormalized untwisted quark mass vanishes, $m_R = 0$.

From the lattice perspective this corresponds to set the bare untwisted mass m_0 to its critical value m_{cr} . The exact way this is achieved is not relevant for what follows, but for a discussion and further references on this topic see [22].

To parametrizes the $O(a)$ uncertainties stemming from the determination of the critical mass, i.e. $m_q = m_0 - m_{\text{cr}} = O(a)$ in the Symanzik effective theory one adds the operator

$$\mathcal{O}_0 = \Lambda^2\bar{\psi}(x)\psi(x), \quad (6.11)$$

where Λ^2 is some energy scale squared which depends on the way the critical mass is determined, e.g. it could be of the order of the QCD scale Λ_{QCD}^2 , or it could be something proportional to $\Lambda_{\text{QCD}}\mu_q$. This allows to check if potential $O(a)$ uncertainties in the critical mass contradict the property of automatic $O(a)$ improvement.

The proof of automatic $O(a)$ improvement for correlation functions containing fields at positive flow-time follows the proof for the $t = 0$ case [26–28]. We extend the relevant symmetries for the Lagrange multipliers

$$\mathcal{R}_{5,t}^{1,2} \cdot \begin{cases} \chi(t, x) \rightarrow i\gamma_5\tau^{1,2}\chi(t, x), \\ \bar{\chi}(t, x) \rightarrow \bar{\chi}(t, x)i\gamma_5\tau^{1,2}, \\ \lambda(t, x) \rightarrow -i\gamma_5\tau^{1,2}\lambda(t, x), \\ \bar{\lambda}(t, x) \rightarrow -i\bar{\lambda}(t, x)\gamma_5\tau^{1,2}, \end{cases} \quad (6.12)$$

and

$$\mathcal{D}_t: \begin{cases} V(t, x; \mu) \rightarrow V^\dagger(t, -x - a\hat{\mu}; \mu), \\ \chi(t, x) \rightarrow e^{3i\pi/2} \chi(t, -x), \\ \bar{\chi}(t, x) \rightarrow \bar{\chi}(t, -x) e^{3i\pi/2}, \\ \lambda(t, x) \rightarrow e^{5i\pi/2} \lambda(t, -x), \\ \bar{\lambda}(t, x) \rightarrow \bar{\lambda}(t, -x) e^{5i\pi/2}. \end{cases} \quad (6.13)$$

The equivalent transformations for continuum fields, that with abuse of notation we indicate in the same way, are the same for the fermion fields, while for the gauge fields the $\mathcal{D}_t$ transformation is $B_\mu(t, x) \rightarrow -B_\mu(t, -x)$. In the $\mathcal{D}_t$ transformation we do not reverse the sign in the t direction because the flow-time has a space–time dimension of 2. Thus any derivative with respect to the flow-time contained in a generic operator will not change the parity related to its dimensionality. To include the twisted mass in the counting of the dimensions of the operators appearing in the lattice and continuum Lagrangian one introduces the spurionic symmetry

$$\tilde{\mathcal{D}}_t = \mathcal{D}_t \times [\mu_q \rightarrow -\mu_q]. \quad (6.14)$$

The lattice action (6.1) at the boundary, and (4.9) in the bulk is invariant under the $\mathcal{R}_{5,t}^{1,2} \times \tilde{\mathcal{D}}_t$ transformation. If the target continuum theory has a vanishing renormalized untwisted mass, $m_R = 0$, it is invariant separately under the $\mathcal{R}_{5,t}^{1,2}$ and the $\tilde{\mathcal{D}}_t$ transformations. This immediately implies that all the higher-dimensional operators in the Symanzik expansion contributing to S_1 are odd under $\mathcal{R}_{5,t}^{1,2}$. This is not true for operators proportional to the untwisted quark mass, but the maximal twist condition $m_R = 0$ forces them to contribute to higher orders in the Symanzik expansion. For example the new terms $\mathcal{O}_2$ and $\mathcal{O}_8$, containing at least one Lagrange multiplier are odd under $\mathcal{R}_{5,t}^{1,2}$, thus they vanish once inserted in $\mathcal{R}_{5,t}^{1,2}$ even correlation functions. The same argument applies for the higher-dimensional operators appearing in the effective theory representations of local operators such as axial currents or pseudoscalar densities at positive flow-time.

Let us see with specific examples how this works. The list of operators contributing at $\mathcal{O}(a)$ to the axial current A_μ^a in the Symanzik effective theory is given by

$$\begin{aligned} (\delta A_\mu^a)_1 &= \partial_\mu P^a(0, x), & (\delta A_\mu^a)_2 &= \tilde{A}_\mu^a(0, x), \\ (\delta A_\mu^a)_3 &= m A_\mu^a(x), & (\delta A_\mu^a)_4 &= \mu_q \epsilon^{3ab} V_\mu^b(x), \end{aligned} \quad (6.15)$$

where

$$\tilde{A}_\mu^a(0, x) = \bar{\lambda}(0, x) \gamma_\mu \gamma_5 \frac{T^a}{2} \psi(x) + \bar{\psi}(x) \gamma_\mu \gamma_5 \frac{T^a}{2} \lambda(0, x). \quad (6.16)$$

It is easy to check that all these operators have opposite $\mathcal{R}_{5,t}^{1,2}$ parity with respect to A_μ^a . The only exception being the term proportional to the untwisted mass m that vanishes at maximal twist. Consistently also the $\tilde{\mathcal{D}}_t$ parity is different between A_μ^a and the higher-dimensional operators. This means that their contribution to the effective correlator vanishes if the continuum limit of the lattice correlator containing A_μ^a is $\mathcal{R}_{5,t}^{1,2}$ even.

Another example is given by the local operator $\tilde{P}^a$. The list of operators contributing at $\mathcal{O}(a)$ in the Symanzik effective theory is given by

$$\begin{aligned} (\delta \tilde{P}^a)_1 &= \partial_\mu \tilde{A}_\mu^a(0, x), & (\delta \tilde{P}^a)_2 &= \hat{P}^a(0, x), \\ (\delta \tilde{P}^a)_3 &= m \tilde{P}^a(0, x), & (\delta \tilde{P}^a)_4 &= \mu_q \epsilon^{3ab} \bar{S}^b(0, x), \end{aligned} \quad (6.17)$$

where

$$\hat{P}^a(0, x) = \bar{\lambda}(0, x) \gamma_5 \frac{T^a}{2} \lambda(0, x). \quad (6.18)$$

As before all the higher-dimensional operators have opposite $\mathcal{R}_{5,t}^{1,2}$ parity with respect to $\tilde{P}^a$, excluding the term proportional to m that anyhow vanishes at maximal twist.

6.2. Chiral condensate

As an application of the WIs we have derived, following the strategy suggested by Lüscher in [2], we show how to compute the chiral condensate with Wtm fermions at maximal twist, retaining the property of multiplicative renormalization and absence of mixing with lower-dimensional operators. Additionally with Wtm at maximal twist one does not need to compute any improvement coefficient but having leading $O(a^2)$ effects discretization errors.

In the basis we have chosen for the fermion fields, the so-called twisted basis, the quark condensate at positive flow-time is related to the expectation value of P^3

$$\Sigma_t = \frac{\Sigma_t^{uu} + \Sigma_t^{dd}}{2} = -i \langle P^3(t, x) \rangle, \quad (6.19)$$

that renormalizes multiplicatively with Z_χ . To relate the Σ_t to the physics of pions we use the VWIs at vanishing and positive flow-time (5.9) and as external probe operator at positive flow-time we choose a pseudoscalar density, i.e.

$$\left\{ \begin{aligned} & \langle [\partial_\mu V_{\mu,R}^1(0, x) + 2\mu_R P_R^2(0, x) + \bar{S}_R^1(0, x)] P_R^2(t, y) \rangle = 0, \\ & \langle [\partial_s \bar{S}^1(s, x) + \partial_\mu \mathcal{V}_\mu^1(s, x)] P_R^2(t, y) \rangle = i \langle P^3(t, y) \rangle \delta(t - s) \delta(x - y). \end{aligned} \right. \quad (6.20)$$

Following the same strategy we have used in Section 4 we integrate the first VWI over space–time and the second one over space–time and over the flow-time direction from 0 to $T > t$. We then obtain

$$2\mu_R \int d^D x \langle P_R^2(0, x) P_R^2(t, y) \rangle = i \langle P_R^3(t, y) \rangle. \quad (6.21)$$

This equation relates the charged pion correlation function with the chiral condensate at positive flow-time. The existence of a conserved vector current guarantees that we can choose the normalization of twisted mass such that $\mu_R P_R^2$ is renormalization group invariant. This insures that Eq. (6.21) is valid with bare correlators up to discretization errors. Automatic $O(a)$ improvement guarantees that the leading discretization errors are of $O(a^2)$. Using the standard VWI with an external probe at vanishing flow-time

$$\langle [\partial_\mu V_{\mu,R}^1(0, x) + 2\mu_R P_R^2(0, x)] P_R^2(0, y) \rangle = 0, \quad x \neq y, \quad (6.22)$$

and considering the spectral decomposition of the charged pseudoscalar correlators we obtain for the renormalized chiral condensate

$$\Sigma_R = \lim_{\mu_R \rightarrow 0} Z_P \frac{\Sigma_t G_\pi}{G_{\pi,t}}, \quad (6.23)$$

where G_π and $G_{\pi,t}$ are the vacuum-to-pion matrix elements of the charged pseudoscalar density respectively at vanishing and positive flow-time. Given that the renormalization between Σ_t and $G_{\pi,t}$ simplifies the only renormalization constant needed to compute the chiral condensate is Z_P .

It is not surprising that we reproduce the same equation obtained by Lüscher in [2]. The additional advantage of using Wtm at maximal twist is automatic $O(a)$ improvement and the fact that there is no need to compute any improvement coefficient. In fact the expectation value $i\langle P^3(t, x) \rangle$ is even under $\mathcal{R}_{5,t}^{1,2}$ as the charged pseudoscalar correlators thus the chiral condensate not only renormalizes multiplicatively but it is also not affected by any $O(a)$ cutoff effects.

With standard or clover Wilson fermions to remove completely $O(a)$ cutoff effects it is necessary to add an additional counterterm to the lattice action proportional to $\bar{\lambda}\lambda$. The tunable coefficient of this term has been labeled in [2] $c_{\bar{\lambda}}$. We can write the quark condensate lattice correlator with the insertion of this term

$$\begin{aligned} & \langle \bar{u}(t, x) \gamma_5 u(t, x) - \bar{d}(t, x) \gamma_5 d(t, x) \rangle \\ &= -a^8 \sum_{y,z} \langle \text{Tr} \{ K(t, x; 0, y) \gamma_5 [S_u(y, z) - ac_{\bar{\lambda}} \delta_{y,z}] K(t, x; 0, z)^\dagger \} \\ & \quad - \text{Tr} \{ K(t, x; 0, y) \gamma_5 [S_d(y, z) - ac_{\bar{\lambda}} \delta_{y,z}] K(t, x; 0, z)^\dagger \} \rangle_G, \end{aligned} \quad (6.24)$$

where $\langle \rangle_G$ indicates the gauge average including the fermionic determinant. The terms proportional to $c_{\bar{\lambda}}$ are independent of the flavor and they cancel out. This is just a reflection of the different $\mathcal{R}_{5,t}^{1,2}$ parities between the observable and the $O(a)$ term.

7. Concluding remarks

The gradient flow is becoming an important tool to probe in interesting ways the non-perturbative dynamic of QCD, one aspect being the non-perturbative renormalization of local fields. The example of the chiral condensate shows that mixing with lower-dimensional operators can be avoided if we relate the quark condensate defined at positive and zero flow-time. A key role for this relation to hold is played by chiral Ward identities.

In this work we have shown that it is possible to use local chiral variations to derive the corresponding Ward identities with operators located at positive flow-time reproducing the identities obtained by Lüscher [2]. While this alternative derivation is interesting on its own, it is also useful when considering more complicated operators. In fact Ward identities can be used to give non-perturbative definitions to the coefficients appearing in small flow-time expansions.

We have then considered the gradient flow in combination with twisted mass fermions. We have shown that the property of automatic $O(a)$ improvement for Wilson twisted mass fermions at maximal twist is still valid at positive flow-time. Using the vector Ward identity derived for twisted mass fermions we find a definition for the chiral condensate that not only is multiplicatively renormalizable but also automatic $O(a)$ improved.

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Appendix A. Charge conjugation symmetry

The charge conjugation symmetry transformation takes the same form for the fields at vanishing flow-time, at positive flow time and the Lagrange multipliers. Here we indicate generically the fermion field as $\phi = \{\psi(0, x), \chi(t, x), \lambda(t, x)\}$ and the corresponding $\bar{\phi}$. For charge conjugation we have

$$C: \begin{cases} V(t, x; \mu) \rightarrow V(t, x; \mu)^*, \\ \phi \rightarrow C^{-1} \bar{\phi}^T, \\ \bar{\phi} \rightarrow -\phi^T C, \end{cases} \quad (\text{A.1})$$

where $V(t, x; \mu)$ is the gauge link at positive flow-time and C satisfies

$$-\gamma_\mu^T = C \gamma_\mu C^{-1}, \quad \gamma_5 = C \gamma_5 C^{-1}. \quad (\text{A.2})$$

Appendix B. Derivation of Eq. (3.15)

In this appendix we derive Eq. (3.15) that we rewrite here for convenience

$$\begin{aligned} & \frac{1}{\mathcal{Z}_{\chi, \lambda}} \int \mathcal{D}[\chi, \bar{\chi}] \mathcal{D}[\lambda, \bar{\lambda}] \mathcal{O}[\bar{\lambda}(s, x) \Gamma^a(s, x) + \bar{\Gamma}^a(s, x) \lambda(s, x)] \exp\{-S_{F, \Pi}\} \\ &= \int_s^\infty dt \int d^D z \left[\bar{\Gamma}^a(s, x) \bar{J}(t, z; s, x) \frac{\delta \mathcal{O}}{\delta \bar{\chi}(t, z)} \right. \\ & \quad \left. + \Gamma^a(s, x) J(t, z; s, x) \frac{\delta \mathcal{O}}{\delta \chi(t, z)} \right]_0, \end{aligned} \quad (\text{B.1})$$

where

$$\mathcal{Z}_{\chi, \lambda} = \int \mathcal{D}[\chi, \bar{\chi}] \mathcal{D}[\lambda, \bar{\lambda}] \exp\{-S_{F, \Pi}\}, \quad (\text{B.2})$$

and the index 0 indicates that the r.h.s. of Eq. (B.1) has to be evaluated with fields χ and $\bar{\chi}$ solutions of the GF equations.

The proof is based on the observation that, given the form of the bulk action, an operator linear in λ or $\bar{\lambda}$, as in the l.h.s. of Eq. (B.1), can be generated by a suitable change of variable. The non-singlet nature of the transformation parametrized by the functions Γ^a and $\bar{\Gamma}^a$ guarantees that the Jacobian of this change of variable has unit determinant.

We start considering the kernel $K(t, z; s, x)$ defined as solution of

$$\begin{cases} (\partial_t - \Delta_z) K(t, z; s, x) = 0, & t > s, \\ \lim_{t \rightarrow s^+} K(t, z; s, x) = \delta(z - x), \\ K(t, z; s, x) = 0, & t < s. \end{cases} \quad (\text{B.3})$$

The Jacobians J and $\bar{J}$ defined in Eq. (3.10) satisfy the same equations. This can be checked applying the gradient flow operator to J and $\bar{J}$ and recalling that in the Jacobians the fields χ and $\bar{\chi}$ are solutions of the gradient flow equations.

We now consider the expectation value of a generic operator $\mathcal{O}$ defined at positive flow-time and function of the fermion or gauge fields. We assume that $\mathcal{O}$ is independent of the Lagrange multipliers. In the functional integral that defines the expectation value we perform the following change of variable

$$\delta\chi(t, z) = i \int_0^t ds \int d^4x \Gamma^a(s, x) K(t, z; s, x) \alpha^a(s, x), \quad (\text{B.4})$$

$$\delta\bar{\chi}(t, z) = i \int_0^t ds \int d^4x \bar{\Gamma}^a(s, x) K(t, z; s, x)^\dagger \alpha^a(s, x). \quad (\text{B.5})$$

As we will show below the Jacobian of this change of variable is one, thus the variation of the expectation value of $\mathcal{O}$ should vanish. Similarly to what happens when deriving Ward identities this implies that $\langle \delta\mathcal{O} \rangle = \langle \mathcal{O} \delta S \rangle$.

The variation of the action according to Eqs. (B.4), (B.5) is given by

$$i \frac{\delta S}{\alpha^a(t, y)} = -[\bar{\lambda}(t, y) \Gamma^a(t, y) + \bar{\Gamma}^a(t, y) \lambda(t, y)]. \quad (\text{B.6})$$

If we consider now that the kernels K and $K^\dagger$ coincide with the Jacobians in Eq. (3.10) computing the variation of the operators $\langle \delta\mathcal{O} \rangle$ we obtain the desired formula (B.1).

We are left to show that the Jacobian of the transformation (B.4), (B.5) has determinant equal to one. From the definition (B.4), (B.5) and given that we consider a transformation with infinitesimal α^a this is a result of the non-singlet nature of the transformation, i.e. of the fact the matrices Γ^a and $\bar{\Gamma}^a$ are traceless.

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