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Lattice QCD with a chirally twisted mass term

ALPHA
Collaboration

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ABSTRACT: Lattice QCD with Wilson quarks and a chirally twisted mass term represents a promising alternative regularization of QCD, which does not suffer from unphysical fermion zero modes. We show how the correlation functions of the renormalized theory are related to the theory with a standard parameterization of the mass term. In particular we discuss the conditions under which these relations take the same form as obtained from naive continuum considerations. We discuss in detail some applications and comment on potential benefits and problems of this framework.

KEYWORDS: Lattice Quantum Field Theory, Lattice Gauge Field Theories, Lattice QCD.

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1. Introduction

Lattice QCD with Wilson quarks [1] is widely used to compute hadronic observables and matrix elements from first principles. It is a gauge invariant regularization with an ultra-local action and an exact global flavour symmetry, but all axial symmetries are explicitly broken by the Wilson term. The latter fact is usually not considered a fundamental problem, as chiral symmetry can be restored by introducing appropriate counterterms. Well-known examples are the additive quark mass

renormalization, the renormalization of the non-singlet axial current and the mixing pattern of the $\Delta S = 2$ effective weak hamiltonian. The corresponding scale independent renormalization constants can be determined both in perturbation theory and non-perturbatively, by imposing continuum chiral Ward identities as normalization conditions [2, 3].

As a result chiral symmetry is restored up to cutoff effects, and the problem has thus been solved from a field theoretical point of view. However, the absence of an exact chiral symmetry has further consequences in practical applications, as it implies that the Wilson-Dirac operator is not protected against zero modes. This is not a problem in principle, as the functional integral over Grassmann variables cannot diverge. After integration over the quark fields, a small eigenvalue of the Wilson-Dirac operator appears both in the fermionic determinant and in the quark propagators entering the correlation functions. Fermi statistics then implies that the limit of a vanishing eigenvalue is always regular. Despite this fact, numerical simulations with some of the standard algorithms may still experience technical problems. In particular, one may suspect that accidental zero modes are at the origin of long autocorrelation times which have been observed in numerical simulations with the hybrid Monte Carlo algorithm [4].

A conceptual problem arises in the so-called quenched approximation, which consists in neglecting the fermionic determinant. The contribution of a small eigenvalue to a fermionic correlator is then not balanced by the determinant, leading to large fluctuations in some of the observables which completely compromise the ensemble average [5]. Gauge field configurations where this happens are called “exceptional” and various recipes of how to deal with them have appeared in the literature [6]–[8]. Strictly speaking, the quenched approximation with Wilson fermions is ill-defined, as the absence of zero modes is only guaranteed for rather heavy quarks. We emphasise that this problem is common to all lattice regularizations with Wilson type fermions. However, its practical relevance in a given physical situation depends on all the details of the chosen lattice action, and on the statistics one would like to achieve in numerical simulations. For example, with non-perturbatively $O(a)$ improved Wilson quarks [9, 5] and the standard Wilson plaquette action, the problem is felt when the quark masses become somewhat lighter than the strange quark’s mass [10]. If the quark mass is further decreased, the frequency of (near-) exceptional configurations strongly increases. As the problem becomes even more pronounced with increasing lattice volume [5], it is clear that the approach to the chiral limit with Wilson type quarks is limited by the zero mode problem rather than by finite volume effects.

To solve the aforementioned practical and conceptual problems we propose to add a non-standard mass term to the (improved) Wilson quark action. The lattice Dirac operator for two quark flavours then reads

$$D_{\text{tmQCD}} = D_W + m_0 + i\mu_q \gamma_5 \tau^3, \quad (1.1)$$

where D_W denotes the massless Wilson-Dirac operator and m_0 is the standard bare quark mass. Further, μ_q which multiplies a term with non-trivial flavor structure (τ^3 is a Pauli matrix acting in flavour space) is referred to as the twisted mass parameter. This action first appeared in a paper of Aoki [11], who introduced the twisted mass term in order to probe the phase structure of the pure Wilson theory. Later, Aoki and Gocksch [12] realized the important property that the Dirac operator (1.1) has no zero modes (for $\mu_q \neq 0$). It is thus a method to regulate the exceptional configurations in a satisfactory field-theoretical way. In ref. [13] the action was briefly mentioned in this context, however implying a limiting procedure $\mu_q \rightarrow 0$ at the end, as μ_q was considered an unphysical parameter. In contrast, our proposal, first presented in [14],¹ is to interpret this theory as an alternative regularization of QCD with two mass degenerate quarks, where the physical quark mass is determined by a combination of both mass parameters. In particular, at finite physical quark mass the twisted mass parameter remains finite too, and the zero mode problem is solved with no need for an extrapolation. We will refer to this approach as QCD with a chirally twisted mass term, or twisted mass QCD (tmQCD) for short.

Since tmQCD is renormalizable by power counting and classically related to QCD by a non-singlet axial transformation of the quark fields, there is little doubt that tmQCD is equivalent to QCD at the quantum level. Furthermore the axial rotation of the fundamental fields induces a mapping between composite fields. One may hence think of this transformation as a change of variables which leaves the physical content of the theory unchanged.

In this paper we want to make precise the correspondence between tmQCD and QCD with standard quark mass parameterization at the level of the renormalized correlation functions and discuss the implications of this correspondence for the case of lattice tmQCD with Wilson quarks. To this end we first regularize both tmQCD and standard QCD using Ginsparg-Wilson quarks (section 2). In this framework the bare correlation functions can be related by a change of variables in the functional integral. Renormalization will be discussed in section 3, in particular we identify renormalization schemes which preserve the relations between the bare correlation functions. Based on universality, it will then be clear how to proceed if the regularization does not respect chiral symmetry, and we discuss in detail the case of Wilson quarks (section 4). We conclude with a few remarks concerning current and future work on tmQCD (section 5).

2. Twisted mass QCD and Ginsparg-Wilson quarks

We start with classical continuum considerations, and then discuss the regularization with Ginsparg-Wilson fermions. In particular we use a formulation which hides the

¹The project was however initiated in 1997.

lattice peculiarities as much as possible, so that naive continuum relations carry over essentially unchanged to the lattice regularized theory.

2.1 Classical continuum theory

We consider the continuum limit of the twisted mass QCD action,²

$$S_F[\psi, \bar{\psi}] = \int d^4x \bar{\psi} (\not{D} + m + i\mu_q \gamma_5 \tau^3) \psi, \quad (2.1)$$

where $D_\mu = \partial_\mu + G_\mu$ denotes the covariant derivative in a given gauge field G_μ , and τ^3 is the third Pauli matrix acting in flavour space. The axial transformation

$$\psi' = \exp(i\alpha \gamma_5 \tau^3 / 2) \psi, \quad \bar{\psi}' = \bar{\psi} \exp(i\alpha \gamma_5 \tau^3 / 2), \quad (2.2)$$

leaves the form of the action invariant, and merely transforms the mass parameters

$$m' = m \cos(\alpha) + \mu_q \sin(\alpha), \quad (2.3)$$

$$\mu'_q = -m \sin(\alpha) + \mu_q \cos(\alpha). \quad (2.4)$$

In particular, the standard action with $\mu'_q = 0$ is obtained if the rotation angle α satisfies the relation

$$\tan \alpha = \mu_q / m. \quad (2.5)$$

Chiral symmetry of the massless action leads to the definition of the Noether currents,

$$A_\mu^a = \bar{\psi} \gamma_\mu \gamma_5 \frac{\tau^a}{2} \psi, \quad V_\mu^a = \bar{\psi} \gamma_\mu \frac{\tau^a}{2} \psi, \quad (2.6)$$

which are only partially conserved at non-zero mass parameters. More precisely, the so-called PCAC and PCVC relations take the form

$$\partial_\mu A_\mu^a = 2m P^a + i\mu_q \delta^{3a} S^0, \quad (2.7)$$

$$\partial_\mu V_\mu^a = -2\mu_q \varepsilon^{3ab} P^b, \quad (2.8)$$

where we have defined the pseudo-scalar and scalar densities,

$$P^a = \bar{\psi} \gamma_5 \frac{\tau^a}{2} \psi, \quad S^0 = \bar{\psi} \psi. \quad (2.9)$$

The axial transformation of the quark and anti-quark fields induces a transformation of the composite fields. For example, the rotated axial and vector currents read,

$$A'^a_\mu \equiv \bar{\psi}' \gamma_\mu \gamma_5 \frac{\tau^a}{2} \psi' = \begin{cases} \cos(\alpha) A_\mu^a + \varepsilon^{3ab} \sin(\alpha) V_\mu^b & (a = 1, 2), \\ A_\mu^3 & (a = 3), \end{cases} \quad (2.10)$$

$$V'^a_\mu \equiv \bar{\psi}' \gamma_\mu \frac{\tau^a}{2} \psi' = \begin{cases} \cos(\alpha) V_\mu^a + \varepsilon^{3ab} \sin(\alpha) A_\mu^b & (a = 1, 2), \\ V_\mu^3 & (a = 3), \end{cases} \quad (2.11)$$

²We adhere to the convention that γ -matrices are hermitian, $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$, with μ, ν, \dots ranging from 0 to 3, and we set $\gamma_5 = \gamma_0 \gamma_1 \gamma_2 \gamma_3$.

and similarly, the rotated pseudo-scalar and scalar densities are given by

$$P'^a = \begin{cases} P^a & (a = 1, 2), \\ \cos(\alpha)P^3 + i \sin(\alpha)\frac{1}{2}S^0 & (a = 3), \end{cases} \quad (2.12)$$

$$S'^0 = \cos(\alpha)S^0 + 2i \sin(\alpha)P^3. \quad (2.13)$$

It is easy to verify that the rotated currents and densities satisfy the PCAC and PCVC relations (2.7), (2.8), with the transformed parameters m' (2.3) and μ'_q (2.4). In particular these relations assume their standard form,

$$\partial_\mu A'^a_\mu = 2m'P'^a, \quad \partial_\mu V'^a_\mu = 0, \quad (2.14)$$

if α is related to the mass parameters as in eq. (2.5).

Finally, we note that the tmQCD and standard QCD actions are exactly related by the transformation (2.2) and therefore share all the symmetries. However, in the chirally twisted basis the symmetry transformations may take a somewhat unusual form. For example, a parity transformation is realized by

$$\psi(x) \longrightarrow \gamma_0 \exp(i\alpha\gamma_5\tau^3)\psi(x_0, -\mathbf{x}), \quad (2.15)$$

$$\bar{\psi}(x) \longrightarrow \bar{\psi}(x_0, -\mathbf{x}) \exp(i\alpha\gamma_5\tau^3)\gamma_0, \quad (2.16)$$

and similar expressions can be obtained for the isospin and the remaining discrete symmetries. It is then straightforward to infer the behaviour of composite fields under these transformations.

2.2 Ginsparg-Wilson quarks

We now replace continuous euclidean space time by a hyper-cubic lattice with spacing a , and we choose some standard lattice action for the gauge fields. The precise choice will not be important in the following, but for definiteness we may take Wilson's original plaquette action. As for the quark fields we assume that the lattice Dirac operator satisfies the Ginsparg-Wilson relation [15],

$$D\gamma_5 + \gamma_5 D = aD\gamma_5 D. \quad (2.17)$$

This relation arises naturally in the construction of fixed point actions [16], and an explicit solution for D has been given by Neuberger [17]. In the following we assume that D is a local operator [18] which satisfies eq. (2.17) and has the conjugation property $D^\dagger = \gamma_5 D \gamma_5$. It then follows that the matrix [19],

$$\hat{\gamma}_5 \stackrel{\text{def}}{=} \gamma_5(1 - aD), \quad (2.18)$$

is hermitian and unitary. The massless action of a quark doublet

$$S_F = a^4 \sum_x \bar{\psi} D \psi, \quad (2.19)$$

has a global $SU(2) \times SU(2)$ invariance [20] which can be parameterised by the transformation

$$\begin{aligned}\psi' &= \exp(i\omega_V^a \tau^a / 2) \exp(i\omega_A^b \hat{\gamma}_5 \tau^b / 2) \psi, \\ \bar{\psi}' &= \bar{\psi} \exp(i\omega_A^a \gamma_5 \tau^a / 2) \exp(-i\omega_V^b \tau^b / 2).\end{aligned}\tag{2.20}$$

Here $\omega_{V,A}^a$ ($a = 1, 2, 3$) are real parameters, τ^a are the Pauli matrices acting on the flavour indices, and repeated indices are summed over. Note that these transformations have the same form as in the continuum, except for the appearance of $\hat{\gamma}_5$. To mask this difference we follow refs. [21, 19] and define left handed fields

$$\psi_L = \frac{1}{2}(1 - \hat{\gamma}_5)\psi, \quad \bar{\psi}_L = \bar{\psi} \frac{1}{2}(1 + \gamma_5),\tag{2.21}$$

and analogously the right handed fields with the complementary projectors. The massless action splits into left and right handed parts due to the identity

$$\bar{\psi} D\psi = \bar{\psi}_L D\psi_L + \bar{\psi}_R D\psi_R,\tag{2.22}$$

and the transformation rules for the chiral fields are exactly as in the continuum. In particular it is straightforward to construct composite fields which transform among each other under a chiral transformation. Examples are the isosinglet scalar and the isovector pseudo-scalar densities which may be defined through

$$S^0 \equiv \bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L = \bar{\psi} \left(1 - \frac{1}{2} aD\right) \psi\tag{2.23}$$

$$P^a \equiv \bar{\psi}_L \frac{\tau^a}{2} \psi_R - \bar{\psi}_R \frac{\tau^a}{2} \psi_L = \bar{\psi} \gamma_5 \frac{\tau^a}{2} \left(1 - \frac{1}{2} aD\right) \psi.\tag{2.24}$$

One finds

$$S'^0 \equiv S^0[\psi', \bar{\psi}'] = \cos(\omega_A) S^0 + 2i \sin(\omega_A) u_A^a P^a,\tag{2.25}$$

where ω_A denotes the modulus of the vector $(\omega_A^1, \omega_A^2, \omega_A^3)$, and $u_A^a = \omega_A^a / \omega_A$ is a unit vector. Similarly, P'^a can be expressed as a linear combination of S^0 and P^a , and we have thus found a multiplet of bare lattice operators transforming under the lattice symmetry in the same way as their continuum counterparts. To define the Ginsparg-Wilson regularization of tmQCD we now use the scalar and pseudo-scalar densities for the mass terms, i.e. we write

$$S_F = a^4 \sum_x [\bar{\psi} D\psi + mS^0 + 2i\mu_q P^3].\tag{2.26}$$

From the preceding discussion it is then clear that the transformation

$$\psi' = \exp(i\beta \hat{\gamma}_5 \tau^3 / 2) \psi, \quad \bar{\psi}' = \bar{\psi} \exp(i\beta \gamma_5 \tau^3 / 2),\tag{2.27}$$

does not change the form of the action, as it corresponds to the special choices $\omega_V^a = 0$ and $\omega_A^a = \beta \delta^{3a}$ in eq. (2.20). Its effect can thus be absorbed in a change of the parameters as in eqs. (2.3), (2.4) with angle β , and the standard QCD action is recovered if $\beta = \alpha$ with α defined as in (2.5).

2.3 Functional integral

We are now prepared to define the functional integral of lattice regularized tmQCD with Ginsparg-Wilson quarks. Denoting the sum of the Wilson plaquette and the fermionic action by S , the partition function is defined by

$$\mathcal{Z} = \int D[\bar{\psi}, \psi] D[U] e^{-S}. \tag{2.28}$$

The physical content of the theory can be extracted from its correlation functions, i.e. n -point functions of the form

$$\langle O(x_1, \dots, x_n) \rangle = \mathcal{Z}^{-1} \int D[\psi, \bar{\psi}] D[U] e^{-S} O(x_1, \dots, x_n), \tag{2.29}$$

where $O(x_1, \dots, x_n)$ is a product of local gauge invariant composite fields which are localised at the space time points x_1, \dots, x_n . In the following we will sometimes indicate the functional dependence upon the quark and anti-quark fields in square brackets, i.e. we set $O \equiv O[\psi, \bar{\psi}]$.

If one restricts the theory to a finite physical space time volume, e.g. by imposing periodic boundary conditions, the functional integral at fixed lattice spacing is a well defined finite dimensional integral, and it is then possible to perform a change of variables of the form (2.27). As the transformation matrices are special unitary, the jacobian is unity. Since the form of the action is preserved by this change of variables, the whole effect is a transformation of the parameters in the action and of the composite fields, viz.

$$\langle O(x_1, \dots, x_n) \rangle_{(m, \mu_q)} = \langle \tilde{O}(x_1, \dots, x_n) \rangle_{(m', \mu'_q)}. \tag{2.30}$$

Here the field \tilde{O} is implicitly defined through

$$\tilde{O}[\psi', \bar{\psi}'] = O[\psi, \bar{\psi}], \tag{2.31}$$

with the transformed quark and anti-quark fields in eq. (2.27). The subscript of the expectation values reminds us of the transformations of the parameters in the action as in eqs. (2.3), (2.4) but with angle β . Eq. (2.30) is an exact identity and defines the starting point for the statement of the aforementioned equivalence between the renormalized theories.

In order to prepare the ground for the discussion of the renormalization procedure we proceed a little further. First we notice that the combination

$$(m')^2 + (\mu'_q)^2 = m^2 + \mu_q^2, \tag{2.32}$$

is left invariant by the chiral rotation, so that it is convenient to use polar mass coordinates,

$$m = M \cos(\alpha), \quad \mu_q = M \sin(\alpha), \tag{2.33}$$

with radial mass M and the angle α chosen according to eq. (2.5). Second, as the bare theory has an exact chiral symmetry, it is useful to decompose operators in multiplets which transform irreducibly under the chiral flavour symmetry transformation. We will denote the irreducible components of the composite fields by $\phi_{kA}^{(r)}(x)$, where r labels the representation, k identifies the multiplet and A labels the members of the multiplet. The general $SU(2) \times SU(2)$ transformation (2.20) is then represented by a matrix $R^{(r)}$, viz.

$$\phi_{kA}^{(r)}[\psi', \bar{\psi}'] = R_{AB}^{(r)}(\boldsymbol{\omega}_V; \boldsymbol{\omega}_A) \phi_{kB}^{(r)}[\psi, \bar{\psi}]. \quad (2.34)$$

Simple examples are the multiplets of the scalar and pseudo-scalar densities, $(\frac{1}{2}S^0, iP^a)$, and of the currents $(\bar{\psi}_L \gamma_\mu \frac{\tau^a}{2} \psi_L, \bar{\psi}_R \gamma_\mu \frac{\tau^a}{2} \psi_R)$.

Without loss of generality we may restrict attention to n -point functions of such fields, and the identity (2.30) then takes the form

$$\begin{aligned} & \left\langle \phi_{k_1 A_1}^{(r_1)}(x_1) \cdots \phi_{k_n A_n}^{(r_n)}(x_n) \right\rangle_{(M, \alpha)} = \\ & = \left\{ \prod_{i=1}^n R_{A_i B_i}^{(r_i)}(-\beta) \right\} \left\langle \phi_{k_1 B_1}^{(r_1)}(x_1) \cdots \phi_{k_n B_n}^{(r_n)}(x_n) \right\rangle_{(M, \alpha - \beta)}, \end{aligned} \quad (2.35)$$

where we have used polar mass coordinates in the subscript, and the shorthand notation

$$R^{(r)}(\beta) \equiv R^{(r)}(\mathbf{0}; 0, 0, \beta), \quad (2.36)$$

for the rotation induced by the axial $U(1)$ transformation (2.27). Note that we may choose the angle β independently of α , and with the choice $\beta = \alpha$ the r.h.s. of eq. (2.35) consists of correlation functions with the standard QCD parameterisation of the mass term.

2.4 Ward identities

Symmetries in Quantum Field Theories are usually expressed in terms of the Ward identities which follow from infinitesimal symmetry transformations. This has the advantage that identities are obtained between correlation functions which are defined within the same theory, even in the presence of explicit breaking terms. To derive the Ward identities we start by introducing the space-time dependent variations of the quark and anti-quark fields,

$$\begin{aligned} \delta_A^a(\omega) \psi(x) &= \omega(x) \frac{\tau^a}{2} (\hat{\gamma}_5 \psi)(x), & \delta_A^a(\omega) \bar{\psi}(x) &= \bar{\psi}(x) \gamma_5 \frac{\tau^a}{2} \omega(x), \\ \delta_V^a(\omega) \psi(x) &= \omega(x) \frac{\tau^a}{2} \psi(x), & \delta_V^a(\omega) \bar{\psi}(x) &= -\bar{\psi}(x) \frac{\tau^a}{2} \omega(x), \end{aligned} \quad (2.37)$$

with some real-valued function $\omega(x)$. The action on arbitrary composite fields is defined by treating the variations like ordinary derivatives. The variation of the action (2.26) then yields

$$\begin{aligned}\delta_A^a(\omega)S &= -a^4 \sum_x \omega(x) \{ \partial_\mu^* A_\mu^a(x) - 2mP^a(x) - i\mu_q \delta^{3a} S^0(x) \}, \\ \delta_V^a(\omega)S &= -a^4 \sum_x \omega(x) \{ \partial_\mu^* V_\mu^a(x) + 2\mu_q \varepsilon^{3ab} P^b(x) \},\end{aligned}\tag{2.38}$$

with the pseudoscalar and scalar densities as defined above, and where the divergences of the symmetry currents are given by

$$\begin{aligned}\partial_\mu^* A_\mu^a(x) &= \left(1 - \frac{am}{2}\right) \left\{ \bar{\psi}(x) \frac{\tau^a}{2} (D\hat{\gamma}_5\psi)(x) - (\bar{\psi}D)(x) \frac{\tau^a}{2} (\hat{\gamma}_5\psi)(x) \right\} + \\ &+ \frac{i}{4} a\mu_q \left\{ \bar{\psi}(x) \tau^3 \tau^a (D\psi)(x) - (\bar{\psi}D\hat{\gamma}_5)(x) \tau^3 \tau^a (\hat{\gamma}_5\psi)(x) \right\},\end{aligned}\tag{2.39}$$

$$\begin{aligned}\partial_\mu^* V_\mu^a(x) &= \left(1 - \frac{am}{2}\right) \left\{ \bar{\psi}(x) \frac{\tau^a}{2} (D\psi)(x) - (\bar{\psi}D)(x) \frac{\tau^a}{2} \psi(x) \right\} + \\ &+ \frac{i}{4} a\mu_q \left\{ \bar{\psi}(x) \tau^3 \tau^a (D\hat{\gamma}_5\psi)(x) - (\bar{\psi}D\hat{\gamma}_5)(x) \tau^3 \tau^a \psi(x) \right\}.\end{aligned}\tag{2.40}$$

Note that these expressions vanish exactly upon summation over x , so that the existence of the currents is guaranteed by the lattice Poincaré lemma [22]. The symmetry currents themselves will not be needed in the following. Explicit expressions for the massless case can be found in [23], for example, but one should keep in mind that the integration of eqs. (2.39), (2.40) is ambiguous by terms with vanishing divergence.

The Ward identities now take the generic form

$$\langle (\delta_X^a(\omega)S) \mathcal{O} \rangle = \langle \delta_X^a(\omega)\mathcal{O} \rangle, \quad X = A, V,\tag{2.41}$$

where \mathcal{O} denotes some product of local composite fields. This is an exact identity, as the space-time dependent change of variables can be made in the functional integral. However, the variation of the composite fields does not exactly transform members of a given multiplet among each other.³ Rather there are extra terms, which arise due to the non-trivial space-time structure of $\hat{\gamma}_5$. For instance, the axial variation of the pseudo-scalar density is given by

$$\delta_A^a(\omega)P^b(y) = \frac{1}{2} \delta^{ab} \omega(y) S^0(y) + \frac{1}{8} a \bar{\psi}(y) \tau^b \tau^a \gamma_5 ([\omega, D] \hat{\gamma}_5 \psi)(y).\tag{2.42}$$

We now first assume that ω is non-zero only in a single lattice point $x \neq y$. Eq. (2.42) then reduces to

$$\delta_A^a(\omega)P^b(y) = -\frac{1}{8} a \omega(x) \bar{\psi}(y) \tau^b \tau^a \gamma_5 D(y, x) (\hat{\gamma}_5 \psi)(x),\tag{2.43}$$

³We thank L. Giusti for drawing our attention to this problem. Although this was known in the literature (cf. e.g. [23]) it has been overlooked by us in an earlier version of this paper.

where $D(y, x)$ denotes the kernel of the Ginsparg-Wilson Dirac operator. Locality of the Ginsparg-Wilson action then implies that the r.h.s. of eq. (2.43) is exponentially small as long as the distance between x and y is large in lattice units. We find that this structure is generic and therefore conclude that the bare PCAC and PCVC relations hold up to exponentially small corrections, provided all operators in the correlation function keep a large distance (in lattice units) from the space-time region where the action is varied.

We now assume that ω is constant in a space-time region R ,

$$\omega(x) = \begin{cases} 1, & \text{if } x \in R \\ 0, & \text{otherwise,} \end{cases} \quad (2.44)$$

which leads to

$$\delta_A^a(\omega)P^b(y) = \begin{cases} \frac{1}{2}\delta^{ab}S^0(y) + \frac{1}{8}a^5 \sum_{x \notin R} \bar{\psi}(y)\gamma_5\tau^b\tau^a D(y, x)(\hat{\gamma}_5\psi)(x), & \text{if } y \in R, \\ -\frac{1}{8}a^5 \sum_{x \in R} \bar{\psi}(y)\gamma_5\tau^b\tau^a D(y, x)(\hat{\gamma}_5\psi)(x), & \text{if } y \notin R, \end{cases} \quad (2.45)$$

Again, locality of the action implies that the extra terms are exponentially small in both cases, provided one has

$$\min_{x \in R} \|x - y\| \gg a, \quad \text{if } y \notin R \quad (2.46)$$

$$\min_{x \notin R} \|x - y\| \gg a, \quad \text{if } y \in R. \quad (2.47)$$

Furthermore, we note that the above example of the pseudoscalar density is generic as the difference to naive continuum considerations always consists of terms involving the lattice Dirac operator. Up to exponentially small corrections, the bare Ward identities (2.41) can therefore be written in the continuum like form

$$\begin{aligned} a^4 \sum_{x \in R} \left\langle (\partial_\mu^* A_\mu^a(x) - 2mP^a(x) - i\mu_q \delta^{3a} S^0(x)) \prod_{i=1}^n \phi_{k_i A_i}^{(r_i)}(x_i) \right\rangle = \\ = -i \sum_{i|x_i \in R} \left(T_A^{(r_i)} \right)_{A_i B}^a \left\langle \phi_{k_1 A_1}^{(r_1)}(x_1) \cdots \phi_{k_i B}^{(r_i)}(x_i) \cdots \phi_{k_n A_n}^{(r_n)}(x_n) \right\rangle, \end{aligned} \quad (2.48)$$

$$\begin{aligned} a^4 \sum_{x \in R} \left\langle (\partial_\mu^* V_\mu^a(x) + 2\mu_q \varepsilon^{3ab} P^b(x)) \prod_{i=1}^n \phi_{k_i A_i}^{(r_i)}(x_i) \right\rangle = \\ = -i \sum_{i|x_i \in R} \left(T_V^{(r_i)} \right)_{A_i B}^a \left\langle \phi_{k_1 A_1}^{(r_1)}(x_1) \cdots \phi_{k_i B}^{(r_i)}(x_i) \cdots \phi_{k_n A_n}^{(r_n)}(x_n) \right\rangle, \end{aligned} \quad (2.49)$$

where we have assumed the conditions (2.46), (2.47) to hold with y replaced by x_i , for all $i = 1, \dots, n$. We have omitted the subscript (M, α) of the correlation functions,

and the expansion,

$$R_{AB}^{(r)}(\boldsymbol{\omega}_V; \boldsymbol{\omega}_A) = \delta_{AB} - \omega_V^a \left(T_V^{(r)}\right)_{AB}^a - \omega_A^a \left(T_A^{(r)}\right)_{AB}^a + \mathcal{O}(\omega^2), \quad (2.50)$$

defines the anti-hermitian generators of infinitesimal $SU(2) \times SU(2)$ rotations in the representation r .

3. Equivalence between the renormalized theories

We discuss under which conditions the identity (2.35) holds in terms of renormalized correlation functions. Without loss one may restrict attention to correlation functions of composite fields which keep a physical distance from each other.

3.1 Renormalized tmQCD

So far we have dealt with the theory at fixed lattice spacing a , and it is not obvious that the theory has a continuum limit. We assume that infrared divergences of the correlation functions are properly taken care of e.g. by working in a finite volume with a suitable choice of boundary conditions. Note that this also ensures analyticity of the correlation functions in the mass parameters. However, we expect that our conclusions will be valid more generally.

In perturbation theory, it has been shown that lattice QCD with Ginsparg-Wilson quarks is renormalizable [24], and we shall assume that this remains true beyond perturbation theory. While this result has been obtained for massless QCD, we do not expect any additional complication here, as both twisted and standard mass terms can be viewed as super-renormalizable interaction terms which do not modify the power counting.

The entire physical information of QCD is contained in the correlation functions of gauge invariant composite fields. Having introduced the lattice regularized path integral and assuming non-perturbative renormalizability, we may completely avoid gauge fixing, and we may also avoid the renormalization of the fundamental fields, which only play the rôle of integration variables. We are thus left with the renormalization of the bare parameters of the action, and the renormalization of the composite fields which enter the correlation functions. The symmetries of the lattice regularized theory are the same as in the continuum except for the continuous space-time symmetry being replaced by the symmetry group of the hyper-cubic lattice. It then follows that renormalized parameters take the form,

$$g_R^2 = Z_g g_0^2, \quad m_R = Z_m m, \quad \mu_R = Z_\mu \mu_q, \quad (3.1)$$

where the renormalization constants are functions,

$$Z = Z(g_0^2, a\mu, \mu_q/\mu, m/\mu), \quad (3.2)$$

and μ denotes the renormalization scale.

Even though chiral symmetry is also broken by the mass terms it is customary to renormalize operators such that the chiral multiplet structure of the massless theory carries over to the renormalized theory. Renormalized operators then are of the form

$$(\phi_R)_{kA}^{(r)} = Z_k \left(\phi_{kA}^{(r)} + c_{kk';AA'}^{(r,r')} a^{d_{k'} - d_k} \phi_{k'A'}^{(r')} \right), \quad (3.3)$$

where d_k and $d_{k'}$ are the mass dimensions of the fields in the multiplets k and k' . The structure of this equation follows from the well-known result of renormalization theory which states that composite fields mix under renormalization with all fields of equal or lower dimension, which transform identically under all the symmetries of the regularized theory. We assume here that $d_{k'} < d_k$, i.e. either there is no mixing with fields of equal mass dimensions, or this has already been taken into account by choosing a basis where the renormalization matrix is diagonal at the renormalization scale μ . Hence the c -coefficients in eq. (3.3) only multiply operators with lower dimensions, and this implies that they cannot depend on the renormalization scale μ [25]. While the multiplicative renormalization constants Z_k are of the form (3.2), the c -coefficients may thus be considered functions of the bare parameters, g_0^2 , $a\mu$ and $a\mu_q$. Note that the multiplet structure of the bare theory is respected by the assignment of a common renormalization constant to all members of a multiplet.

In the following we shall assume that the renormalization of the theory and the composite fields works out along these lines. While this is guaranteed in perturbation theory, the non-perturbative renormalization of power divergent operators may require an additional effort. In particular, it may be necessary to first implement Symanzik's improvement programme to sufficiently high order in the lattice spacing a before the power divergences can be subtracted in an unambiguous way.

3.2 A special choice of renormalization scheme

We would like to identify renormalization schemes where the equation (2.35) carries over to the renormalized theory, with renormalized fields of the form (3.3). First of all, we notice that the exact PCAC and PCVC relations of the bare theory imply that μ_q and m can be renormalized by the same renormalization constant. We may thus choose $Z_m = Z_\mu$ implying a multiplicative renormalization of the bare radial mass M by the same constant. Furthermore, α is not renormalized as it is determined by the ratio of the mass parameters. As the effect of the chiral rotation is a change of α , we would like to choose all multiplicative renormalization constants independently of this angle, i.e.

$$Z = Z(g_0^2, a\mu, M/\mu). \quad (3.4)$$

A simple example is a mass-independent renormalization scheme which is obtained by renormalizing the theory in the chiral limit [26]. As we have assumed an infrared regularization to be in place, such renormalization schemes do exist and it

is then obvious that eq. (2.35) holds for the renormalized correlation functions of multiplicatively renormalizable operators, viz.

$$\begin{aligned} & \left\langle (\phi_{\mathbf{R}})_{k_1 A_1}^{(r_1)}(x_1) \cdots (\phi_{\mathbf{R}})_{k_n A_n}^{(r_n)}(x_n) \right\rangle_{(M_{\mathbf{R}}, \alpha)} = \\ & = \left\{ \prod_{i=1}^n R_{A_i B_i}^{(r_i)}(-\beta) \right\} \left\langle (\phi_{\mathbf{R}})_{k_1 B_1}^{(r_1)}(x_1) \cdots (\phi_{\mathbf{R}})_{k_n B_n}^{(r_n)}(x_n) \right\rangle_{(M_{\mathbf{R}}, \alpha - \beta)}. \end{aligned} \quad (3.5)$$

The expectation values in the renormalized theory are defined as in the bare theory, except that the bare parameters are expressed in terms of the renormalized parameters $M_{\mathbf{R}}$ and $g_{\mathbf{R}}$. Note that eq. (3.5) is again an exact identity, if this is true for (2.35) and provided the renormalization constants are chosen exactly as specified above (i.e. not only up to cutoff effects).

The case of power divergent operators is slightly more complicated. In general, if eq. (3.5) is to be satisfied the c -coefficients cannot be independent of α . For example, the renormalized scalar and pseudo-scalar densities are of the form

$$i(P_{\mathbf{R}})^a = Z_{\mathbf{P}} (iP^a + \delta^{a3} a^{-3} c_{\mathbf{P}}), \quad (3.6)$$

$$\frac{1}{2}(S_{\mathbf{R}})^0 = Z_{\mathbf{S}} \left(\frac{1}{2}S^0 + a^{-3} c_{\mathbf{S}} \right), \quad (3.7)$$

with $Z_{\mathbf{S}} = Z_{\mathbf{P}}$, and it is well-known that $c_{\mathbf{P}}$ vanishes at $\mu_{\mathbf{q}} = 0$.

Rather than being independent of α , the additive counterterms satisfy a covariance condition. More precisely, assuming that all multiplicative renormalization constants are of the form (3.4), the requirement that eqs. (2.35) and (3.5) hold simultaneously implies,

$$R_{AB}^{(r)}(-\beta) c_{kk';BC}^{(r,r')}(g_0^2, aM, \alpha - \beta) = c_{kk';AB}^{(r,r')}(g_0^2, aM, \alpha) R_{BC}^{(r')}(-\beta), \quad (3.8)$$

where only the index B is summed, all others being fixed. In the example of the pseudo-scalar and scalar densities one finds the equations

$$\begin{pmatrix} c_{\mathbf{P}}(\alpha) \\ c_{\mathbf{S}}(\alpha) \end{pmatrix} = \begin{pmatrix} \cos \beta & \sin \beta \\ -\sin \beta & \cos \beta \end{pmatrix} \begin{pmatrix} c_{\mathbf{P}}(\alpha - \beta) \\ c_{\mathbf{S}}(\alpha - \beta) \end{pmatrix}, \quad (3.9)$$

where we have only indicated the dependence upon the angle. It is obvious that $c_{\mathbf{P}}^2 + c_{\mathbf{S}}^2$ is independent of α and due to the vanishing of $c_{\mathbf{P}}(0)$, the solution can be parameterised as follows,

$$c_{\mathbf{P}}(\alpha) = c_{\mathbf{S}}(0) \sin(\alpha), \quad c_{\mathbf{S}}(\alpha) = c_{\mathbf{S}}(0) \cos(\alpha). \quad (3.10)$$

In other words, if the renormalization problem for the scalar density can be solved in standard QCD, the solution at all other values of α is given by these equations.

3.3 Differential equation in α

The requirements for the renormalization scheme are best characterised by a differential equation in α . We start by considering the third flavour component of the axial Ward identity (2.48), chose the region R to be the space-time manifold itself and obtain the *exact* identity of the bare theory,

$$\begin{aligned} \frac{\partial}{\partial\alpha} \Big|_{M,g_0} \left\langle \prod_{i=1}^n \phi_{k_i A_i}^{(r_i)}(x_i) \right\rangle_{(M,\alpha)} &= \\ &= \sum_{i=1}^n T_{A_i B}^{(r_i)} \left\langle \phi_{k_1 A_1}^{(r_1)}(x_1) \cdots \phi_{k_i B}^{(r_i)}(x_i) \cdots \phi_{k_n A_n}^{(r_n)}(x_n) \right\rangle_{(M,\alpha)}, \end{aligned} \quad (3.11)$$

where $T^{(r)} \equiv (T_A^{(r)})^3$. Note in particular that the normalising factor of the path integral is independent of α and hence does not generate a disconnected contribution.

Next we recall that analyticity of the renormalized correlation functions in the mass parameters m_R and μ_R is guaranteed by the infrared cutoff. Therefore, also their derivative with respect to α must exist, as the relation

$$\frac{\partial}{\partial\alpha} \Big|_{M_R, g_R} = m_R \frac{\partial}{\partial\mu_R} \Big|_{m_R, g_R} - \mu_R \frac{\partial}{\partial m_R} \Big|_{\mu_R, g_R}, \quad (3.12)$$

follows directly from the definition of the (renormalized) polar mass coordinates [cf. eq. (2.33)]. Differentiating a renormalized n -point function at fixed renormalized parameters, applying the chain rule and using eq. (3.11), one obtains the differential equation,

$$\begin{aligned} \left(\nabla_\alpha - \sum_{i=1}^n l_{k_i} \right) \left\langle (\phi_R)_{k_1 A_1}^{(r_1)}(x_1) \cdots (\phi_R)_{k_n A_n}^{(r_n)}(x_n) \right\rangle_{(M_R, \alpha)} &= \\ &= \sum_{i=1}^n T_{A_i B}^{(r_i)} \left\langle (\phi_R)_{k_1 A_1}^{(r_1)}(x_1) \cdots (\phi_R)_{k_i B}^{(r_i)}(x_i) \cdots (\phi_R)_{k_n A_n}^{(r_n)}(x_n) \right\rangle_{(M_R, \alpha)}. \end{aligned} \quad (3.13)$$

Here the differential operator ∇_α is defined through

$$\nabla_\alpha \stackrel{\text{def}}{=} \frac{\partial}{\partial\alpha} \Big|_{M_R, g_R} + l_M M_R \frac{\partial}{\partial M_R} \Big|_{\alpha, g_R} + l_g g_R^2 \frac{\partial}{\partial g_R^2} \Big|_{\alpha, M_R}, \quad (3.14)$$

and the coefficients are given by

$$l_X = \frac{\partial \log Z_X}{\partial\alpha} \Big|_{M, g_0}, \quad X = M, g, k_1, \dots, k_n. \quad (3.15)$$

With a suitable choice of the irrelevant parts of the renormalization counterterms eq. (3.13) holds exactly at finite lattice spacing. The very existence of the differentiated correlation function then leads to a constraint for the additive counterterms,

viz.

$$\frac{\partial}{\partial \alpha} \Big|_{M, g_0} c_{kk'; AC}^{(r, r')} = \left\{ T_{AB}^{(r)} c_{kk'; BC}^{(r, r')} - c_{kk'; AB}^{(r, r')} T_{BC}^{(r')} \right\}. \quad (3.16)$$

As one might expect, integrating eq. (3.16) from α to $\alpha - \beta$ reproduces the covariance relation (3.8). Note however, that eq. (3.16) holds without assuming eq. (3.4).

To relate the renormalized correlation functions defined at two different values of the angle α one just has to integrate the differential equation (3.13). It is possible to formally write down the general solution. However, we do not find this particularly illuminating and therefore just mention that the general relation is much more complicated than eq. (3.5). The question then arises under which conditions the relation does take the simple form (3.5). For this to work out, the l.h.s. of eq. (3.13) should reduce to the partial derivative with respect to α , i.e. one requires

$$\left[l_M M_R \frac{\partial}{\partial M_R} \Big|_{\alpha, g_R} + l_g g_R^2 \frac{\partial}{\partial g_R^2} \Big|_{\alpha, M_R} - \sum_{i=1}^n l_{k_i} \right] \times \left\langle (\phi_R)_{k_1 A_1}^{(r_1)}(x_1) \cdots (\phi_R)_{k_n A_n}^{(r_n)}(x_n) \right\rangle_{(M_R, \alpha)} = 0. \quad (3.17)$$

Note that such an equation must hold for all renormalized correlation functions. Therefore, unless M_R and g_R are related in a special way, the l_X must all vanish, i.e. the multiplicative renormalization constants all take the form (3.4).

We finally remark that eq. (3.13) expresses the re-parameterisation invariance of the theory: an infinitesimal change of quark variables of the form (2.27) is compensated by a change of α , M_R and g_R . Our derivation makes use of the axial Ward identity as the change of variables (2.27) corresponds to a special chiral symmetry transformation. However, more general changes of variables can be considered using rather general results of renormalization theory.

3.4 The rôle of the Ward identities

Eq. (3.5) is the relation between renormalized tmQCD and QCD in its simplest form. Its infinitesimal version is eq. (3.13) with vanishing coefficients l_X (3.15). We have argued that it is possible to renormalize the Ginsparg-Wilson regulated theory such that eq. (3.5) holds, and we have worked out the conditions on the renormalization constants in this regularization. Based on universality one thus expects that tmQCD in other, not necessarily chirally invariant regularizations can again be renormalized such that eq. (3.5) is satisfied up to cutoff effects. At least in perturbation theory this can be proved rigorously.

In view of the formulation of tmQCD with Wilson quarks, we would like to emphasise the rôle of the renormalized tmQCD Ward identities, which are of the same form as eqs. (2.48), (2.49). As is well-known, the Ward identities ensure that the

renormalized composite fields form chiral multiplets, and fix the absolute normalization of the symmetry currents. Furthermore, the mass parameters are renormalized inversely to the pseudo-scalar and scalar densities, and this implies that one may set

$$m_R = M_R \cos \alpha, \quad \mu_R = M_R \sin \alpha, \quad (3.18)$$

with the angle α which remains unrenormalized.

We are now going to demonstrate that the renormalized tmQCD Ward identities also imply that certain linear combinations of the correlation functions satisfy the Ward identities of standard QCD. In the following we assume the continuum limit has been taken and use a shorthand notation for the renormalized correlation functions,

$$G \equiv \left\langle (\phi_R)_{kA}^{(r)}(y) \mathcal{O}_{\text{ext}} \right\rangle_{(M_R, \alpha)}, \quad (3.19)$$

where \mathcal{O}_{ext} is some product of renormalized fields which are localized in the exterior of the finite physical space-time region R . Furthermore we assume $y \in R$ and denote by $G_{A,V,P}^a$ and G_S the same correlation functions with an insertion of $\partial_\mu (A_R)_\mu^a$, $\partial_\mu (V_R)_\mu^a$, $(P_R)^a$ and $(S_R)^0$ at the space-time point x , integrated over the region R with respect to x . The renormalized Ward identities may then be written in the form

$$\begin{aligned} G_A^a - 2M_R \{ \cos(\alpha) G_P^a + i \sin(\alpha) \delta^{3a} G_S \} &= -iT_A^a G, \\ G_V^a + 2M_R \sin(\alpha) \varepsilon^{3ab} G_P^b &= -iT_V^a G, \end{aligned} \quad (3.20)$$

where the abbreviation

$$T_X^a G \equiv \left(T_X^{(r)} \right)_{AB}^a \left\langle (\phi_R)_{kB}^{(r)}(y) \mathcal{O}_{\text{ext}} \right\rangle_{(M_R, \alpha)} \quad (3.21)$$

has been used for $X = A, V$.

We now consider the two linear combinations

$$cG_A^1 + sG_V^2 - 2M_R \{ c \cos \alpha + s \sin \alpha \} G_P^1 = -i (cT_A^1 + sT_V^2) G, \quad (3.22)$$

$$cG_V^2 - sG_A^1 - 2M_R \{ c \sin \alpha - s \cos \alpha \} G_P^1 = -i (cT_V^2 - sT_A^1) G. \quad (3.23)$$

Multiplying both sides of the equation by the matrices $R^{(r)}(\alpha)$, setting

$$R_\alpha G \equiv R_{AB}^{(r)}(\alpha) \left\langle (\phi_R)_{kB}^{(r)}(y) \mathcal{O}_{\text{ext}} \right\rangle_{(M_R, \alpha)} \quad (3.24)$$

and also defining

$$G_{A'}^1 \equiv cG_A^1 + sG_V^2, \quad G_{V'}^2 \equiv cG_V^2 - sG_A^1, \quad (3.25)$$

we then find

$$\begin{aligned} R_\alpha G_{A'}^1 - 2M_R \{ c \cos \alpha + s \sin \alpha \} R_\alpha G_P^1 &= -i R_\alpha (cT_A^1 + sT_V^2) G, \\ R_\alpha G_{V'}^2 - 2M_R \{ c \sin \alpha - s \cos \alpha \} R_\alpha G_P^1 &= -i R_\alpha (cT_V^2 - sT_A^1) G. \end{aligned} \quad (3.26)$$

We notice that in order to preserve the canonical normalization of the primed currents, one needs $c^2 + s^2 = 1$, i.e. we may set

$$c = \cos(\alpha'), \quad s = \sin(\alpha'). \quad (3.27)$$

It is then clear that the standard Ward identities can be obtained by choosing $\alpha' = \alpha$, and provided the equations

$$R_{AB}^{(r)}(\alpha) \left(c(T_A^{(r)})_{BC}^1 + s(T_V^{(r)})_{BC}^2 \right) R_{CD}^{(r)}(-\alpha) = (T_A^{(r)})_{AD}^1, \quad (3.28)$$

$$R_{AB}^{(r)}(\alpha) \left(c(T_V^{(r)})_{BC}^2 - s(T_A^{(r)})_{BC}^1 \right) R_{CD}^{(r)}(-\alpha) = (T_V^{(r)})_{AD}^2, \quad (3.29)$$

hold. By differentiating with respect to α and using the Lie algebra of the $SU(2) \times SU(2)$ generators,

$$[T_A^a, T_A^b] = \varepsilon^{abc} T_V^c, \quad [T_A^a, T_V^b] = \varepsilon^{abc} T_A^c, \quad [T_V^a, T_V^b] = \varepsilon^{abc} T_V^c, \quad (3.30)$$

one arrives at the conclusion that eqs. (3.28), (3.29) are indeed satisfied. Note that the same procedure applies to the remaining flavour components of the Ward identities. Hence, the validity of the tmQCD Ward identities implies that

- there exist particular linear combinations of correlation functions which satisfy the standard QCD Ward identities for two degenerate quark flavours with mass M_R ,
- the linear combinations only depend on the angle α , which is determined by the ratio of the quark mass parameters which appear in the Ward identities.

In particular it is clear that the angle α has no physical significance. We may start with any value of α and still obtain the standard chiral flavour Ward identities. As a given theory is identified by its symmetries this implies the equivalence of theories defined at different values of α , provided the remaining symmetries are either α -independent or transform covariantly. This is certainly true on the level of the renormalized composite fields: for any transformation of the composite fields at $\alpha = 0$ one may identify the corresponding transformation in the renormalized twisted theory.

3.5 Concluding remarks

In practical applications one would like to work with tmQCD at a given fixed value of α , and just invoke eq. (3.5) in order to *interpret* the results in terms of standard QCD. According to the above discussion one may start by imposing the tmQCD Ward identities in the renormalized theory. Besides defining the value of α this procedure restores the chiral multiplet structure of the bare theory. One then still needs to impose a renormalization condition per chiral multiplet. If this is done

either in the chiral limit or independently of α , eq. (3.5) provides the relation to the theory defined at any other angle α , including $\alpha = 0$. The simplification in the Ginsparg-Wilson regularization consists in the validity of bare continuum-like tmQCD Ward identities, and in the related fact that the bare Ward identity masses coincide with the bare mass parameters of the action. Finally we stress that the classical continuum theory allows to infer the relation (3.5) between renormalized theories and may hence be used as a guide.

4. Twisted mass QCD with Wilson quarks

In this section we discuss in some detail the regularization with Wilson fermions, including some practical aspects of applications.

4.1 Symmetries of the bare theory

With Wilson quarks the tmQCD Dirac operator is as given in eq. (1.1) with the usual massless Wilson-Dirac operator⁴

$$D_W = \frac{1}{2} \sum_{\mu=0}^3 \left\{ \gamma_\mu (\nabla_\mu + \nabla_\mu^*) - a \nabla_\mu^* \nabla_\mu \right\}. \quad (4.1)$$

For simplicity we defer the discussion of $O(a)$ improved tmQCD to a separate publication [32]. Here we note that the Wilson term is not left invariant by the axial rotation (2.2), and the lattice regulated theories at $\mu_q = 0$ and $\mu_q \neq 0$ are thus different. This is of course welcome as otherwise the zero mode problem would be present in both cases (cf. section 1). One may think of more general lattice Dirac operators, also including a chirally twisted Wilson term. However, a moment of thought reveals that this is not really more general, as an axial rotation (2.2) may then be used in the lattice theory to eliminate the extra Wilson term. Modulo a more general coefficient of the standard Wilson term and with re-defined bare mass parameters, one then obtains again the action corresponding to eq. (1.1).

As compared to the theory with $N_f = 2$ standard Wilson quarks ($\mu_q = 0$) we find that the exact $U(2)$ symmetry is reduced to a $U(1)$ symmetry leading to fermion number conservation, and a vectorial $U(1)$ symmetry with generator $\tau^3/2$. Concerning the space-time symmetries, the lattice action is invariant under axis permutations, whereas reflections such as parity are a symmetry only if combined with either a flavour exchange

$$F : \quad \psi \rightarrow \tau^1 \psi, \quad \bar{\psi} \rightarrow \bar{\psi} \tau^1, \quad (4.2)$$

or a sign change of the twisted mass term $\mu_q \rightarrow -\mu_q$. We will refer to the thus modified parity symmetries as P_F and \tilde{P} respectively. The list of exact symmetries

⁴For unexplained notation and conventions we refer to ref. [27]

is completed by charge conjugation, and we note that twisted mass lattice QCD with Wilson quarks has a positive self-adjoint transfer matrix [32].

4.2 Renormalized parameters

As in section 3 we assume that infrared divergences are regulated e.g. by working in a finite space-time volume with suitable boundary conditions. This implies analyticity of the theory in the mass parameters and it is then rather obvious that twisted mass lattice QCD is renormalizable by power counting [28]. The counterterm structure follows from the symmetries of the regularization. Based on these symmetries one concludes that tmQCD is finite after the usual renormalization of the coupling and the standard mass parameter,

$$g_R^2 = Z_g g_0^2, \quad m_R = Z_m m_q, \quad m_q = m_0 - m_c, \quad (4.3)$$

and, in addition a *multiplicative* renormalization of the twisted mass parameter,

$$\mu_R = Z_\mu \mu_q. \quad (4.4)$$

In particular we note that the modified parity symmetry, P_F , is sufficient to exclude a counterterm $\propto \text{tr}\{F_{\mu\nu}\tilde{F}_{\mu\nu}\}$.

4.3 Ward identities and renormalization of composite fields

Following section 3 we require that the renormalized theory satisfies the axial and vector Ward identities, i.e. the renormalized analogues of eqs. (2.48), (2.49). Concerning the vector Ward identity the situation is the same as with Ginsparg-Wilson fermions, due to the exact flavour symmetry of massless Wilson quarks. Therefore eq. (2.49) holds exactly, with the point-split vector current

$$\begin{aligned} \tilde{V}_\mu^a(x) = \frac{1}{2} \left\{ \bar{\psi}(x)(\gamma_\mu - 1) \frac{\tau^a}{2} U(x, \mu) \psi(x + a\hat{\mu}) + \right. \\ \left. + \bar{\psi}(x + a\hat{\mu})(\gamma_\mu + 1) \frac{\tau^a}{2} U(x, \mu)^{-1} \psi(x) \right\}, \end{aligned} \quad (4.5)$$

and the local pseudo-scalar density. It then follows that the vector current is protected against renormalization, i.e. $Z_{\tilde{V}} = 1$. More generally, the multiplicative renormalization constants of composite fields which belong to the same isospin multiplet must be identical in order to respect the vector Ward identities. An example is the renormalized pseudo-scalar density which has the structure

$$i(P_R)^a = Z_P \{ iP^a + \delta^{a3} a^{-3} c_P \}, \quad (4.6)$$

and c_P vanishes exactly at $\mu_q = 0$. The vector Ward identity here implies that Z_P is the same for all flavour components, and, moreover,

$$Z_P = Z_\mu^{-1}. \quad (4.7)$$

In contrast, the axial Ward identity does not hold in the bare theory. Axial Ward identities therefore provide normalization conditions which determine finite renormalization constants such as Z_A , or finite ratios of scale dependent renormalization constants, such as Z_S/Z_P [2]. Moreover, these finite renormalization constants only depend on the bare coupling g_0 and may therefore be determined in the chiral limit using standard procedures [3]. Note that the finite renormalization constants restore chiral symmetry of the bare theory up to cutoff effects. Once this is achieved the renormalization of multiplicatively renormalizable fields is similar to the Ginsparg-Wilson case, i.e. the renormalization constant for a given multiplet is determined by imposing a renormalization condition on one of its members. Of particular practical interest are mass-independent renormalization schemes, which are obtained by imposing a renormalization condition at $\mu_q = m_q = 0$ [26]. Based on universality we then expect that the relations (3.5) between renormalized correlation functions hold up to cutoff effects. According to section 3 the same can be achieved by imposing α -independent renormalization conditions, where, in the case of Wilson fermions the angle α must be defined through the Ward identity masses (cf. subsection 4.4).

In principle the Ward identities also determine additive renormalization constants which arise due to the explicit breaking of chiral symmetry. An example is the renormalization of the iso-singlet scalar density, which has the same structure as in eq. (3.7), however, with a coefficient c_S which does not vanish in the chiral limit. Therefore, the renormalization of the third axial Ward identity (2.48) requires the explicit subtraction of power divergences. While power divergent renormalization problems do not present any particular difficulty to any finite order of perturbation theory, it is less clear how to proceed in a non-perturbative approach. A general discussion of this topic is beyond the scope of this work. Here we just note that the renormalization of the third axial Ward identity may in fact be avoided if one assumes that the physical isospin symmetry is restored in the renormalized theory. In the following we will make this (plausible) assumption and not discuss the third axial Ward identity any further.

4.4 Definition of the angle α

According to section 3.4 the angle α is uniquely defined through the renormalized Ward identity masses. Assuming that Z_P has been fixed, the renormalized twisted mass parameter is determined due to eq. (4.7). The renormalized axial current and the first two components of the pseudo-scalar density may then be used to define m_R through the renormalized PCAC relation

$$\partial_\mu (A_R)_\mu^a = 2m_R (P_R)^a, \quad a = 1, 2. \quad (4.8)$$

In practice one first defines a bare PCAC mass m from the ratio of correlation functions involving the bare axial current and pseudo-scalar density. The renormalized

PCAC mass is then given by

$$m_R = Z_A Z_P^{-1} m = Z_m m_q. \quad (4.9)$$

Using eq. (4.7), the angle α is then determined as

$$\tan \alpha = \frac{\mu_R}{m_R} = \frac{\mu_q}{Z_A m} = \frac{\mu_q}{Z_m Z_P m_q}. \quad (4.10)$$

In general one thus needs the bare PCAC mass m and the axial current normalization constant Z_A to obtain α . Note that the latter is not needed in the special case $m = 0$, i.e. if $\alpha = \pi/2$.

4.5 Avoiding lattice renormalization problems

Once tmQCD has been renormalized in the way described above, eq. (3.5) can be applied to establish a “dictionary” between the renormalized correlation functions in QCD and tmQCD. For example, the 2-point function of the axial current and the pseudo-scalar density in standard QCD translates as follows

$$\begin{aligned} \langle (A_R)_0^1(x) (P_R)^1(y) \rangle_{(M_R,0)} &= \cos(\alpha) \langle (A_R)_0^1(x) (P_R)^1(y) \rangle_{(M_R,\alpha)} + \\ &+ \sin(\alpha) \langle \tilde{V}_0^2(x) (P_R)^1(y) \rangle_{(M_R,\alpha)}. \end{aligned} \quad (4.11)$$

More generally, relations between the renormalized composite fields can be inferred from the corresponding relations in the classical theory (cf. section 2). In particular, the above example follows from eqs. (2.10)–(2.12).

As tmQCD and standard QCD with Wilson quarks are not related by a lattice symmetry, the counterterm structure for composite fields with the same physical interpretation depends upon α . Given a physical amplitude it may hence be possible that a particular choice of α leads to simplifications. An obvious case is the computation of F_π from the 2-point function (4.11). While the standard approach (i.e. the direct computation of the l.h.s.) requires to first determine the renormalized axial current, the r.h.s. of this equation at $\alpha = \pi/2$ only contains the vector current (4.5) which is protected against renormalization.

Even more interesting is the application of tmQCD to matrix elements of the iso-singlet scalar density. At $\alpha = \pi/2$, the physical scalar density is represented by the third component of the pseudo-scalar density, see eq. (2.13). While the scalar density is cubically divergent even in the chiral limit, the pseudo-scalar density has a quadratic divergence which vanishes *exactly* at $\mu_q = 0$. The situation is therefore comparable to the case of the renormalized scalar density in standard QCD with Ginsparg-Wilson fermions.

4.6 Inclusion of heavier quarks

It is straightforward to generalise tmQCD to include any number of heavier quark flavours. For the latter one may use the standard regularization with (improved) Wilson quarks, as the zero mode problem is practically absent at mass parameters which correspond to the physical strange quark mass. The renormalization procedure can again be carried out such that the chiral flavour Ward identities are respected, which now also involve mixed operators of light and heavy quarks. Hence we expect that the “dictionary” between tmQCD and standard QCD can again be established by naive continuum considerations. As an example we consider the tmQCD continuum action (2.1) and add the action of the strange quark,

$$S_F[\psi, \bar{\psi}, s, \bar{s}] = \int d^4x \{ \bar{\psi} (\not{D} + m + i\mu_q \gamma_5 \tau^3) \psi + \bar{s} (\not{D} + m_s) s \}. \quad (4.12)$$

Using a physical notation,

$$\psi = \begin{pmatrix} u \\ d \end{pmatrix}, \quad \bar{\psi} = (\bar{u} \ \bar{d}), \quad (4.13)$$

the standard PCAC relation,

$$\partial_\mu (\bar{d}' \gamma_\mu \gamma_5 s) = (m' + m_s) \bar{d}' \gamma_5 s, \quad (4.14)$$

is obtained with the rotated axial current and pseudo-scalar density,

$$\bar{d}' \gamma_\mu \gamma_5 s = \cos\left(\frac{1}{2}\alpha\right) \bar{d} \gamma_\mu \gamma_5 s + i \sin\left(\frac{1}{2}\alpha\right) \bar{d} \gamma_\mu s, \quad (4.15)$$

$$\bar{d}' \gamma_5 s = \cos\left(\frac{1}{2}\alpha\right) \bar{d} \gamma_5 s - i \sin\left(\frac{1}{2}\alpha\right) \bar{d} s, \quad (4.16)$$

and with the angle α and the light quark mass m' as given in section 2.1

4.7 Application to the $\Delta S = 2$ effective weak hamiltonian

Also in the case of operators involving light and strange quarks certain renormalization problems of standard Wilson quarks can be circumvented. An interesting example is the $\Delta S = 2$ part of the effective weak hamiltonian,

$$O^{\Delta S=2} = \{ \bar{s} \gamma_\mu (1 - \gamma_5) d \}^2. \quad (4.17)$$

In phenomenology one is mainly interested in the hadronic matrix element of this operator between K_0 and \bar{K}_0 states [29]. As parity does not change in this transition, only the parity conserving part of the operator contributes. Hence one decomposes the operator into parity even and odd parts,

$$O^{\Delta S=2} = O_{VV+AA} - 2O_{VA}. \quad (4.18)$$

In the regularization with Ginsparg-Wilson fermions the operator $O^{\Delta S=2}$ and thus

both O_{VV+AA} and O_{VA} are renormalized multiplicatively. With Wilson quarks, the remaining symmetries imply that O_{VV+AA} mixes with four other parity even operators of the same mass dimension, whereas O_{VA} is still renormalized multiplicatively [30]. In tmQCD we now observe that the parity even operator in the standard basis is represented by the combination

$$O'_{VV+AA} = \cos(\alpha)O_{VV+AA} - 2i \sin(\alpha)O_{VA} . \tag{4.19}$$

In particular, at $\alpha = \pi/2$, only O_{VA} appears on the r.h.s., and one concludes that matrix elements of the physical operator O'_{VV+AA} can be computed in tmQCD without solving the complicated renormalization problem for the parity even operator.⁵ In particular, the $K_0 - \bar{K}_0$ mixing amplitude could be extracted from the 3-point function involving O_{VA} and appropriately rotated interpolating fields for the kaons [cf. eqs. (4.15), (4.16)].

One might be worried that additional counterterms to O_{VA} may be necessary in tmQCD. As there is no such term at $\mu_q = 0$, possible counterterms must be accompanied by at least one power of the twisted mass parameter, and the flavour structure requires them to be again four-quark operators. For dimensional reasons such counterterms can only contribute cutoff effects of the order $a\mu_q$, and a closer look shows that the parity even operators multiplied by $a\mu_q$ are indeed allowed by the tmQCD symmetries.

4.8 Technical complications

The equivalence between tmQCD and standard QCD is a statement about the renormalized theories in the continuum limit. When tmQCD is used to define the standard QCD correlation functions, some of the physical symmetries are only restored in the continuum limit. In particular, this is the case of the flavour symmetry and parity, which are exact lattice symmetries in standard QCD with Wilson fermions, but which are only recovered in the continuum limit if $\alpha \neq 0$. In practice the problem shows up e.g. as an ambiguity in the definition of α , which is induced by the usual ambiguity in the definition of the critical mass m_c by terms of $O(a)$ (or $O(a^2)$ if the theory is improved) [27]. To illustrate the consequences consider the computation of the pion mass at fixed cutoff a , using the 2-point function

$$G(x_0 - y_0) = a^3 \sum_{\mathbf{x}} \langle P'^3(x) P'^3(y) \rangle . \tag{4.20}$$

In tmQCD this correlation function is computed by replacing P'^3 as in eq. (2.12), where the relative multiplicative renormalization of S^0 and P^3 is assumed to have been fixed by the axial Ward identity. Note also that the exponential decay of this correlation can be determined without knowledge of the additive renormalization constants.

⁵For an alternative proposal see ref. [31].

It is now obvious that both the ambiguity in α and the $O(a)$ ambiguity in the relative renormalization of the densities imply that the correlation function (4.20) contains cutoff effects which are proportional to the propagator of the (physical) scalar density S'^0 . An analysis of the 2-point function (4.20) at fixed a must therefore take into account the states with the quantum numbers of an isosinglet scalar state. We note in passing that $O(a)$ improvement does not alter this situation, as it merely reduces the ambiguities to $O(a^2)$. In particular, at fixed cutoff, the relevant symmetries remain inexact and the qualitative behaviour of the 2-point function (4.20) remains unchanged.

In general the analysis of the hadron spectrum in tmQCD at fixed a must include states which are allowed by the lattice symmetries but have the “wrong” continuum quantum numbers. Although this is not a fundamental problem, the analysis is somewhat more complicated than in lattice QCD with standard Wilson quarks. We also note a side effect for the determination of hadronic matrix elements. When these are extracted from tmQCD correlation functions it may not be necessary to increase the distances until the desired physical state is completely isolated. It is sufficient to establish that contributions from the excited states with the correct continuum quantum numbers are negligible, as all other contaminations merely modify the cutoff effects of the matrix element.

5. Conclusions

In this paper we have advocated the use of twisted mass QCD with Wilson quarks as an alternative regularization of QCD with two degenerate light quarks. Using Ginsparg-Wilson fermions as a tool, we have demonstrated in what sense tmQCD is equivalent to standard QCD. In particular, we have clarified under which conditions the relations between renormalized correlation functions take the simple form (3.5), which is the quantum analogue of the naive relations derived in the classical continuum theory.

Twisted mass lattice QCD provides a clean field theoretical solution to the problem of unphysical zero modes. While our work on tmQCD is motivated by this problem, we also observe a few additional benefits. In particular we have given examples where renormalization problems of lattice operators can be circumvented by working in the fully twisted theory with $\alpha = \pi/2$. For the sake of simplicity we did not discuss $O(a)$ improvement of tmQCD. This topic is deferred to a separate publication [32].

First numerical simulations using (quenched) tmQCD have already been carried out, and a scaling test in a small volume has been presented in [33]. It is hoped that the chiral limit can be approached much more closely in tmQCD than previously possible with Wilson quarks. In particular the ALPHA collaboration plans to extend the work of [34] to much smaller quark masses where (quenched) chiral perturbation

theory should be safely applicable [35]. Furthermore, a project to determine the $K_0 - \bar{K}_0$ mixing amplitude using tmQCD is underway [36]. In the future, it will also be interesting to see whether numerical simulations of full QCD can benefit from using a twisted mass term.

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