LATTICE QCD WITH A CHIRAL TWIST

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In these lectures I explain how chiral symmetry of continuum QCD naturally leads to a class of lattice regularisations known as twisted mass QCD (tmQCD). As compared to standard Wilson quarks, its advantages are the absence of unphysical zero modes, the possibility to circumvent lattice renormalisation problems and automatic O(\(a\)) improvement. On the other hand, the physical parity and flavour symmetries are explicitly broken. I discuss these aspects and then turn to the theory in a finite space-time volume with Schrödinger functional boundary conditions. Again, chiral transformations of the continuum theory may be used as a guide to formulate an alternative lattice regularisation of the Schrödinger functional, with interesting applications to renormalization problems in QCD.

1. Introduction

In recent years, twisted mass QCD (tmQCD) has become a popular variant of lattice QCD with Wilson-type quarks \(^1,^2,^3\). Initially designed to render the (partially) quenched approximation well-defined through the elimination of unphysical zero modes, it was soon realised that tmQCD could also be used to circumvent some notorious lattice renormalization problems \(^1,^2\). Later, Frezzotti and Rossi \(^4\) observed that scaling violations in tmQCD can be reduced to O(\(a^2\)) without the need for all the O(\(a\)) counterterms required with standard Wilson quarks (\(a\) being the lattice spacing). This property, referred to as “automatic O(\(a\)) improvement”, has attracted further attention and a number of groups have started large scale numerical simulations using tmQCD. In these lectures I do not attempt to review this work in progress\(^a\). Here I would rather like to give an introduction to the basic con-
cepts. This includes in particular a discussion of $O(a)$ improvement and the question whether it is compromised by currently used non-perturbative renormalization procedures based on the QCD Schrödinger functional (SF-schemes). In fact, the standard Schrödinger functional boundary conditions turn out to be difficult to reconcile with automatic $O(a)$ improvement and the construction of an alternative set-up for the Schrödinger functional may therefore be advantageous.

This writeup is organised as follows: I start with the interplay between the choice of the quark mass term and the form taken by parity, flavour and chiral symmetry transformations (sect. 2). After a reminder of standard Wilson quarks and the problem of unphysical zero modes (section 3), lattice tmQCD is introduced in sect. 4. Based on the formal continuum theory a dictionary between tmQCD and QCD correlation functions is readily established, which is expected to hold between properly renormalised correlation functions. It then becomes clear how to by-pass certain renormalization problems of standard Wilson quarks (sect. 5), and the computation of $B_K$ is discussed in some detail. In sect. 6 automatic $O(a)$ improvement of tmQCD is analysed using Symanzik’s effective theory. Potential problems of tmQCD associated with flavour and parity breaking are shortly mentioned in sect. 7. In sect. 8, the properties of Schrödinger functional renormalisation schemes (SF schemes) are discussed. Motivated by the clash of the standard set-up with automatic $O(a)$ improvement and by the slow decoupling of heavy quarks in mass-dependent SF schemes, a modified definition of the Schrödinger functional is proposed, and its effectiveness regarding $O(a)$ improvement is illustrated in an example taken from perturbation theory. Section 9 contains some conclusions.

2. Continuum QCD and chiral transformations

Let us consider the continuum action of QCD with $N_f = 2$ massless quarks\(^b\). Decomposing the action into a pure gauge and a fermionic part, $S = S_g + S_f$, we here focus on the fermionic part,

$$S_f = \int d^4x \, \bar{\psi}(x) D\psi(x), \quad D = \gamma_\mu D_\mu.$$  \hspace{1cm} (1)

The quark and antiquark fields $\psi, \bar{\psi}$ are flavour doublets, interacting minimally with the gluon field $A_\mu$ via the covariant derivative $D_\mu = \partial_\mu + A_\mu$.

\(^b\)Conventions used for Euclidean $\gamma$-matrices in 4 dimensions: $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$, $\gamma^\dagger_\mu = \gamma_\mu$, where $\mu, \nu = 0, 1, 2, 3$, and $\gamma_5 = \gamma_0 \gamma_1 \gamma_2 \gamma_3$, $\sigma_{\mu\nu} = i[\gamma_\mu, \gamma_\nu]$. 
The massless fermionic action has a global chiral-flavour \( SU(2) \times SU(2) \) invariance, corresponding to the transformations,

\[
\psi' = \exp(i\omega_A^a \tau^a / 2) \psi
\]

\[
\bar\psi' = \bar\psi \exp(-i\omega_A^a \tau^a / 2) \exp(i\omega_V^b \gamma_5 \tau^b / 2) \psi,
\]

where \( \tau^a (a = 1, 2, 3) \) are Pauli matrices, \( \omega^a_A \) are transformation parameters\(^c\). This notation distinguishes the axial from the vector generators (corresponding to the flavour or isospin \( SU(2) \) subgroup) in a standard way.

A quark mass term breaks the chiral flavour symmetry explicitly, leaving only the vector or isospin symmetry intact. The above notation for the symmetry transformations was introduced with the standard quark mass term \( \bar\psi \psi \) in mind, but e.g. the choice

\[
\psi' = \bar\psi \exp(i\omega_A^a \gamma_5 \tau^a) \psi = \cos(\omega_A)\bar\psi \psi + i \sin(\omega_A) u_A^a \bar\psi \gamma_5 \tau^a \psi,
\]

would be completely equivalent. Here, \( \omega_A \) denotes the modulus of \( (\omega_1^A, \omega_2^A, \omega_3^A) \) and \( u_A^a = \omega_A^a / \omega_A \) is a unit vector. In fact, it is only after the introduction of the quark mass term that the distinction between axial and vector symmetries acquires a meaning. By definition, the vector symmetry transformations are those which leave the quark mass term invariant. Similarly, the quark mass term is supposed to be invariant under parity transformations. As a consequence, the form of a symmetry transformation depends on the choice of the mass term. While a standard mass term implies that a parity transformation can be realised as

\[
\psi(x_0, x) \rightarrow \gamma_0 \psi(x_0, -x), \quad \bar\psi(x_0, x) \rightarrow \bar\psi(x_0, -x) \gamma_0,
\]

the alternative choice of (3) for the mass term means that a parity transformation will look more complicated, for instance

\[
\psi(x_0, x) \rightarrow \gamma_0 \exp(i\omega_A^a \gamma_5 \tau^a) \psi(x_0, -x),
\]

\[
\bar\psi(x_0, x) \rightarrow \bar\psi(x_0, -x) \exp(i\omega_A^a \gamma_5 \tau^a) \gamma_0.
\]

Similarly, the isospin transformation obtained with a standard mass term corresponds to (2) with all axial transformation parameters set to zero, \( \omega_A^a = 0 \) (whence the notation), whereas the mass term (3) leads to the much less intuitive formula

\[
\psi \rightarrow \exp(-i\omega_A^a \gamma_5 \tau^a / 2) \exp(i\omega_V^b \gamma_5 \tau^b / 2) \exp(i\omega_A^c \gamma_5 \tau^c / 2) \psi,
\]

\[
\bar\psi \rightarrow \bar\psi \exp(\omega_A^a \gamma_5 \tau^a / 2) \exp(-i\omega_V^b \gamma_5 \tau^b / 2) \exp(-i\omega_A^c \gamma_5 \tau^c / 2),
\]

\(^c\)Summation over repeated indices \( a, b = 1, 2, 3 \) is understood.
where $\omega^b_V (b = 1, 2, 3)$ are transformation parameters while $\omega^a_A (a = 1, 2, 3)$ are again fixed. The situation is reminiscent of the choice of a coordinate system, and our intuition about the form of symmetry transformations is thus based on a particular choice of “field coordinates”. Of course, this raises the question why one should deviate from the standard choice of the mass term. In the continuum and for regularisations preserving chiral symmetry there is indeed no point in introducing a twisted mass term, for any non-standard choice could be brought into the standard form by using an axial rotation, which, being a symmetry of the massless theory, has no further effects. The situation is different in regularisations which break chiral symmetry, such as lattice regularisations with Wilson type quarks. One may then obtain different regularisations of QCD which have equivalent continuum limits but differ at the cutoff level. This will be made more precise a bit later.

3. Standard Wilson quarks

Standard Wilson quarks are characterised by the fermionic lattice action,

$$S_f = a^4 \sum_x \bar{\psi}(x)(D_W + m_0)\psi(x),$$  \hspace{1cm} (7)

$$D_W = 3 \sum_{\mu=0}^3 \left\{ \frac{1}{2}(\nabla_\mu + \nabla^*_\mu)\gamma_\mu - a\nabla^*_\mu\nabla_\mu \right\}. \hspace{1cm} (8)$$

Here, $m_0$ is a bare mass parameter and the covariant lattice derivatives in the Wilson-Dirac operator are defined as usual (see ref. 6 for unexplained notation). Assuming $N_f$ quark flavours the lattice action has an exact $U(N_f)$ vector symmetry, and is invariant under axis permutations, reflections such as parity and charge conjugation. Furthermore, unitarity of lattice QCD with Wilson quarks has been rigorously established 7. These nice properties of standard Wilson quarks come with a price: all axial symmetries are explicitly broken by the last term in eq. (8), called the Wilson term. This has a number of consequences:

1. Linear mass divergence: the quark mass term is not protected against additive renormalization, i.e. any renormalized quark mass is of the form $m_R = Z_m(m_0 - m_{cr})$, where the critical mass is linearly divergent, i.e. $m_{cr} \propto 1/a$.

2. Axial current renormalization: since axial transformations are not an exact symmetry, there is no exact current algebra, and the non-
singlet axial current requires a non-trivial multiplicative renormalization to restore current algebra up to $O(a)$ effects.

(3) Definition of the chiral condensate as expectation value of a local operator: the renormalised iso-singlet scalar density has the structure,

$$\langle \bar{\psi} \psi \rangle_R = Z_{S0} \{ \bar{\psi} \psi + c_S a^{-3} \}.$$  \hspace{1cm} (9)

In a regularisation which respects chiral symmetry, the additive renormalization constant $c_S$ would be proportional to $am$, with $m$ being a multiplicatively renormalisable bare quark mass. This means that the chiral condensate is well-defined in the chiral limit once its multiplicative renormalisation has been carried out. In contrast, with Wilson quarks one first needs to subtract the cubic power divergence, even in the chiral limit.

(4) Cutoff effects: the leading cutoff effects with Wilson-type fermions are proportional to $a$, rather than $a^2$. Again, this is a consequence of chiral symmetry breaking. This is easily seen by looking at the structure of the counterterms which are to be included for the on-shell $O(a)$ improvement of the theory à la Symanzik.

From a field theoretical point of view this illustrates the proliferation of additional counterterms in a case where the regularisation breaks a continuum symmetry. One should note, however, that there is no remaining theoretical or conceptual problem.

### 3.1. Wilson quarks and unphysical fermionic zero modes

Nevertheless, technical problems may arise within the current practice of numerical simulations with Wilson-type quarks. This is related to the fact that, for a given gauge background field, the massive Wilson-Dirac operator $D_W + m_0$ is not protected against zero modes unless the bare mass parameter $m_0$ is positive. However, due to additive quark mass renormalisation, the masses of the light quarks typically correspond to negative bare mass parameters, which leaves the Wilson-Dirac operator unprotected against zero modes in the physically interesting region. These modes are considered unphysical, since one expects from the continuum theory that any non-zero value of the renormalised quark mass prohibits zero modes of the Dirac operator.

It is instructive to look at a typical fermionic correlation function, such
as the pion propagator given by
\[ G^{ab}(x - y) = -\left\langle \bar{\psi}(x) \gamma_5 \tau^a \frac{1}{2} \psi(x) \gamma_5 \tau^b \frac{1}{2} \psi(y) \right\rangle = -Z^{-1} \int D[U, \psi, \bar{\psi}] e^{-S} \bar{\psi}(x) \gamma_5 \tau^a \frac{1}{2} \psi(x) \gamma_5 \tau^b \frac{1}{2} \psi(y), \]
where \( \tau^a, a = 1, 2, 3 \), are the Pauli matrices acting in flavour space and \( Z = \langle 1 \rangle \). It is convenient to introduce the operator,
\[ Q = \gamma_5 (D_W + m_0), \quad Q = Q^\dagger, \]
which acts in single flavour space. Integrating over the quark and anti-quark fields one obtains
\[ G^{ab}(x - y) = \frac{1}{2} \delta^{ab} Z^{-1} \int D[U] e^{-S_g} \text{det}(Q^2) \text{tr} [Q^{-1}(x, y) Q^{-1}(y, x)], \]
where the flavour structure has been reduced analytically and the remaining trace is over colour and spin indices. The important point to notice is that the resulting expression is never singular. Denoting the eigenfunction of \( Q \) for a given eigenvalue \( \lambda_i \) by \( \varphi_i(x) \), the pion propagator takes the form
\[ G^{ab}(x - y) = \frac{1}{2} \delta^{ab} Z^{-1} \int D[U] e^{-S_g} \prod_i \lambda_i^2 \times \sum_{j,k} \lambda_j^{-1} \lambda_k^{-1} \varphi_j(x) \varphi_j^*(y) \varphi_k(x) \varphi_k^*(y). \]

In other words, the eigenvalues in the denominator are always compensated by corresponding factors from the determinant. The limit of vanishing eigenvalues is always regular and a strict lower bound on the eigenvalue spectrum is not required for the theory to be well-defined.

However, the absence of a lower bound on \( |\lambda_i| \) may still lead to technical problems, either due to the use of unphysical approximations or due to the set-up of numerical simulations:

3.1.1. Quenched and partially quenched approximations

As the computational cost for the generation of an ensemble of gauge field configurations is dominated by the inclusion of the quark determinant, a widely used approximation consists in omitting the determinant when taking the average over gauge fields. The quark propagators with the eigenvalues in the denominator may then become singular, and gauge field
configurations where this happens are called “exceptional”. The example in figure 1 taken from \(^8\) shows the ensemble average of the pion propagator over all gauge configurations but a single exceptional one (dashed line), where the propagator deviates dramatically from the average (dots and solid line). The inclusion of the exceptional configuration in the ensemble average would lead to much larger errors, while its omission invalidates the Monte Carlo procedure. In principle one should say that the quenched approximation with Wilson type quarks is ill-defined, since zero modes are bound to occur if the ensemble of gauge configurations is large enough. However, the frequency of near zero modes depends very sensitively upon the bare quark mass and is in fact a function of the lattice size and all the other bare parameters in the lattice action. One may therefore think of the quenched approximation as being operationally defined, if for an ensemble of, say, a few hundred configurations the problem is typically absent. “Safe” parameter ranges may then be quoted for a given action, but this situation is clearly unsatisfactory. In particular, as the problem is not sharply defined, one may always be unlucky and encounter near zero modes even at parameter values which have previously been considered safe. In practice it is this problem which has limited the approach to the chiral limit, rather than finite volume effects due to the pions becoming too light.

Obviously, the problem is expected to disappear once the quark determinant is properly included. Usually this is done by including the complete determinant in the effective gauge field measure used in the importance sampling, and the probability for a gauge configuration to be included in the ensemble becomes proportional to the eigenvalues. Exceptional configurations are then never produced. However, even in this case, one is often interested in varying the valence quark masses independently of the sea quark masses, a situation which is referred to as the partially quenched approximation. One may also have different numbers of valence and sea quarks, or Wilson valence quarks and sea quarks of a different kind. In all these cases one expects similar problems with unphysical zero modes as in the quenched approximation.

3.1.2. Potential problems in the Hybrid Monte Carlo algorithm

Most numerical simulations use some variant of the Hybrid Monte Carlo algorithm \(^9\). Integrating the molecular dynamics trajectories in fictitious phase space then requires the evaluation of the fermionic force term and thus the inversion of the Dirac operator at each step in molecular dynamics.
time. The force term may become very large if an exceptional configuration is encountered, and the molecular dynamics integrator tends to become unstable if the product of the force and the step size exceeds a certain critical value. To avoid this situation one may hence be forced to decrease the step size to very small values thereby increasing the cost of the simulation. It is likely that this problem was at the heart of the difficulties encountered in the past with simulations of Wilson type quarks. However, various developments over the past few years seem to have solved this problem (see for a recent account of current simulation algorithms and cost estimates and for further discussion).

4. Twisted mass lattice QCD

Initially the main motivation for introducing a twisted mass term was the problem with zero modes discussed in the previous section. The lattice action for a doublet $\psi$ of $N_f = 2$ mass degenerate quarks is now given by

$$S_f = a^4 \sum_x \bar{\psi}(x)(D_W + m_0 + i \mu_q \gamma_5 \tau^3)\psi(x),$$

(14)
where $\mu_q$ denotes the bare twisted mass parameter. It is easy to see that the presence of this parameter eliminates any unphysical zero modes, for

$$\det(D_W + m_0 + i\mu_q \gamma_5 \tau^3) = \det \begin{pmatrix} Q + i\mu_q & 0 \\ 0 & Q - i\mu_q \end{pmatrix} = \det (Q^2 + \mu^2_q) > 0.$$  \tag{15}

The difference in the determinant already shows that twisted mass and standard QCD cannot be the same regularisation. In fact, any attempt to perform an axial rotation so as to eliminate the twisted mass term will rotate the Wilson term in eq. (8), too. the equivalence between both regularisations can therefore only be expected to hold in the continuum limit. We will discuss this more in detail below.

Here it suffices to say that the chiral flavour symmetry of twisted mass QCD is reduced to an exact U(1) symmetry with generator $\tau^3/2$. Furthermore, charge conjugation, axis permutations and reflections combined with a flavour permutation, e.g.

$$\psi(x_0, \mathbf{x}) \to \gamma_0 \tau_1 \psi(x_0, -\mathbf{x}), \quad \bar{\psi}(x_0, \mathbf{x}) \to \bar{\psi}(x_0, -\mathbf{x}) \gamma_0 \tau_1,$$  \tag{16}

are exact symmetries. Finally, the construction of a positive and self-adjoint transfer matrix for standard Wilson quarks can be generalised to twisted mass QCD, provided $\mu_q$ is real and the usual condition on the standard bare mass parameter, $|\kappa| < 1/6$, with $\kappa = (2am_0 + 8)^{-1}$ is satisfied \cite{3}.

### 4.1. Equivalence between tmQCD and QCD

Taking the continuum limit, we see that the fermionic continuum action of tmQCD,

$$S_f = \int d^4x \bar{\psi}(x)(\slashed{D} + m + i\mu_q \gamma_5 \tau^3)\psi(x),$$  \tag{17}

can be related to the standard action by a global chiral field rotation,

$$\psi' = R(\alpha)\psi, \quad \bar{\psi}' = \bar{\psi}R(\alpha), \quad R(\alpha) = \exp \left( i\alpha \gamma_5 \frac{\tau^3}{2} \right).$$  \tag{18}

Choosing the angle $\alpha$ such that $\tan \alpha = \mu_q/m$, the action for the primed fields takes the standard form,

$$S'_f = \int d^4x \bar{\psi'}(x)(\slashed{D} + M)\psi'(x), \quad M = \sqrt{m^2 + \mu^2_q}.$$  \tag{19}

In QCD all physical observables can be extracted from gauge invariant correlation functions of composite fields. We would therefore like to study the
relationship between correlation functions in tmQCD and standard QCD. To this end we introduce polar mass coordinates,

\[ m = M \cos(\alpha), \quad \mu = M \sin(\alpha), \]  

and consider the correlation functions labelled by \((M, \alpha)\),

\[ \langle O[\psi, \bar{\psi}] \rangle_{(M, \alpha)} = Z^{-1} \int D[U, \psi, \bar{\psi}] \, O[\psi, \bar{\psi}] \, e^{-S[m, \mu]}, \]  

Treating the functional integral like an ordinary integral we change the variables to \(\psi'\) and \(\bar{\psi}'\) of eq. (18) and re-label these new integration variables to \(\psi\) and \(\bar{\psi}\) afterwards. In this way we arrive at the identity,

\[ \langle O[\psi, \bar{\psi}] \rangle_{(M, \alpha)} = \langle O[R(\alpha)\psi, \bar{R}(\alpha)] \rangle_{(M, \alpha)} \cdot \]  

To go a step further, we now assume that the functional \(O[\psi, \bar{\psi}]\) consists of factors which are members of a chiral multiplet. Considering such a field \(\phi^{(r)}_A[\psi, \bar{\psi}]\) in the representation \(r\), the transformation of \(\psi\) and \(\bar{\psi}\) by \(R(\alpha)\) induces the transformation of \(\phi^{(r)}_A\) by \(R^{(r)}(\alpha)\) in the representation \(r\),

\[ \phi^{(r)}_A[R(\alpha)\psi, \bar{R}(\alpha)] = R^{(r)}_{AB}(\alpha) \phi^{(r)}_B[\psi, \bar{\psi}]. \]  

For \(n\)-point functions of such fields, one obtains the identity,

\[ \langle \phi^{(r_1)}_{A_1} \cdots \phi^{(r_n)}_{A_n} \rangle_{(M, 0)} = \left( \prod_{i=1}^n R^{(r_i)}_{A_i B_i}(\alpha) \right) \langle \phi^{(r_1)}_{B_1} \cdots \phi^{(r_n)}_{B_n} \rangle_{(M, \alpha)}. \]  

The correlation functions in standard QCD labelled by \((M, 0)\) are just linear combinations of those in twisted mass QCD, labelled by \((M, \alpha)\). The inverse relation can be obtained by inverting the matrices \(R^{(r)}(\alpha)\). This is trivial, as the axial rotation (18) forms an abelian subgroup of the chiral flavour group, so that \([R^{(r)}(\alpha)]^{-1} = R^{(r)}(-\alpha)\). Examples of chiral multiplets are the non-singlet currents \((A^a_\mu, V^a_\mu)\) or the non-singlet axial density combined with the singlet scalar density, \((\frac{1}{2} S^0, P^a)\). In terms of quark fields one has

\[ A^a_\mu = \bar{\psi} \gamma_\mu \gamma_5 \frac{3}{2} \psi, \quad V^a_\mu = \bar{\psi} \gamma_\mu \frac{3}{2} \psi, \quad P^a = \bar{\psi} \psi, \quad S^0 = \bar{\psi}\psi, \]  

and one may then easily infer the transformation behaviour of these chiral multiplets:

\[ A^a_1 = c A^1_\mu + s V^2_\mu, \quad A^a_2 = c A^2_\mu - s V^1_\mu, \quad A^a_3 = A^3_\mu, \quad P^a = P^a, \quad (a = 1, 2), \quad V^1_\mu = c V^1_\mu + s A^2_\mu, \quad V^2_\mu = c V^2_\mu - s A^1_\mu, \quad V^3_\mu = V^3_\mu, \quad S^0 = c S^0 + 2 i s P^3, \]  

(26)
Here the notation \( O' \equiv O[\psi', \bar{\psi}'] \), \( c \equiv \cos(\alpha) \), \( s \equiv \sin(\alpha) \) was used. For a correlator of \( A^1_\mu(x) \) and \( P^1(y) \) in standard QCD this means

\[
\langle A^1_\mu(x) P^1(y) \rangle_{(M,0)} = \cos(\alpha) \langle A^1_\mu(x) P^1(y) \rangle_{(M,\alpha)} + \sin(\alpha) \langle V^2_\mu(x) P^1(y) \rangle_{(M,\alpha)}.
\]  

(27)

In other words, eqs. (26) relate an insertion of the primed fields into standard QCD correlators to the insertion of the corresponding r.h.s. into tmQCD correlators. In particular, we note that the PCAC and PCVC relations in the physical basis

\[
\partial_\mu A^a_\mu = 2M P^a, \quad \partial_\mu V^a_\mu = 0,
\]

(28)

are equivalent to linear combinations of their twisted counterparts,

\[
\partial_\mu A^a_\mu = 2m P^a + \delta^{3a} i \mu_q S^0, \\
\partial_\mu V^a_\mu = -2\mu_q \epsilon^{3ab} P^b.
\]

(29)

In conclusion, the formal continuum theory provides us with a dictionary between correlation functions in standard and twisted mass QCD. However, all these considerations have been quite formal, and we need to specify how such a dictionary carries over to the renormalized theories.

### 4.2. Beyond the formal continuum theory

To clarify this question let us suppose that tmQCD is regularised on the lattice with Ginsparg-Wilson quarks, where chiral and flavour symmetries are the same as in the continuum. Identities such as Eqs. (24) may then be derived in the bare theory. If in addition, we start from a finite volume with, say, periodic boundary conditions for all fields, the functional integral becomes a finite dimensional Grassmann integral. Therefore, these identities are no longer formal, but on firm mathematical grounds, and all one has to show is that the renormalisation procedure can be carried out such that they continue to hold in the renormalised theory. This is straightforward, as one just has to make sure that all members of a given chiral multiplet are renormalised in the same way, and that the multiplicative renormalization constants do not depend on the twist angle \( \alpha \). This can be achieved e.g. by imposing renormalisation conditions in the massless limit. Hence, in this case, the dictionary introduced above holds between the renormalised correlation functions of both theories. Assuming universality to hold beyond perturbation theory, this establishes the equivalence of both versions of QCD at the non-perturbative level, since any other
regularisation, chirally symmetric or not, will then lead to the same renormalised correlation functions up to cutoff effects. While there is no reason to doubt that universality holds generally, one should be aware that it has rigorously been established only in perturbation theory and for selected regularisations (e.g. lattice regularisations with Wilson type quarks).

4.3. Lattice tmQCD with Wilson quarks

In tmQCD on the lattice with Wilson quarks the axial transformation relating continuum tmQCD to standard QCD is not an exact symmetry. Therefore, equivalence can only be expected to hold in the continuum limit, i.e. for properly renormalized correlation functions and up to cutoff effects. The lattice symmetries imply the counterterm structure, with the following result for the renormalised parameters,

\[ g_R^2 = Z g_0^2, \quad m_R = Z_m (m_0 - m_{cr}), \quad \mu_R = Z\mu_q. \]

(30)

It is a priori not obvious how the twist angle \( \alpha \) should be defined from the mass parameters. The key observation is that chiral symmetry can be restored in the bare lattice theory up to cutoff effects, by imposing axial Ward identities as normalisation conditions\(^\text{15}\). This fixes the relative renormalization of all members of a chiral multiplet, such as \( Z_A/Z_V \) for the symmetry currents\(^d\), or \( Z_{S^0}/Z_P \) for the iso-triplet axial and the iso-inglet scalar densities. Note that such ratios are scale independent functions of \( g_0 \) only, which are expected to converge to 1 in the continuum limit with a rate \( g_0^2 \propto -1/\ln a \). In particular, these ratios do not depend upon the quark mass parameters and may therefore be determined in the massless limit\(^\text{16}\) where the tmQCD and standard QCD actions coincide. The connection between the mass parameters and chiral Ward identities is established by choosing renormalisation schemes such that the PCAC and PCVC relations hold, with the renormalised currents and and axial density, and the renormalised mass parameters. The renormalization constants may then be shown to satisfy the identities, \( Z_m = Z_{S^0}^{-1} \) and \( Z_\mu = Z_P^{-1} \). With these conventions it is clear that the ratio of renormalised mass parameters is known once the critical mass and the ratio \( Z_{S^0}/Z_P \) are given,

\[ \tan \alpha = \frac{\mu_R}{m_R} = \frac{Z_{S^0}}{Z_P} \frac{\mu_q}{m_0 - m_{cr}}. \]

(31)

\(^d\) \( Z_V = 1 \) only holds if the (partially) conserved point-split vector current \( \tilde{V}_\mu^a \) is used.
Besides the ratio of renormalization constants one thus needs to determine the critical mass. In practice this can be done by measuring a bare PCAC mass $m$ from correlation functions with some external field $O$,

$$m = \frac{\langle \partial_\mu A_\mu(x) O \rangle}{\langle P^1(x) O \rangle},$$  

(32)

and by using the relation

$$m_R = Z_p^{-1} Z_A m, \quad m = Z_A^{-1} Z_m Z_P (m_0 - m_{ct}).$$  

(33)

Alternatively one may use the measured bare PCAC quark mass $m$ to obtain $\alpha$ directly,

$$\tan \alpha = \mu_q / (ZA m),$$  

(34)

provided one has previously determined $ZA$. Already at this point one notes that the choice $\alpha = \pi/2$ is special, as in this case one merely needs to determine the critical mass. The choice $\alpha = \pi/2$ is referred to a full or maximal twist, because the physical quark mass is then entirely defined by the twisted mass parameter $\mu_q$.

Having determined the twist angle, and the relative renormalizations within chiral multiplets, chiral symmetry is restored up to cutoff effects for the correlation functions of members of these multiplets. In a second step one just needs to make sure that this property of the bare theory is not compromised by the renormalization procedure, i.e. one is in a similar situation as in the bare theory with Ginsparg-Wilson quarks. Proceeding in the same way, the formal identities of subsect. 4.1 will hold in the renormalised theory.

An important point to notice is that the twist angle $\alpha$ is a new parameter which reflects the freedom to choose a direction in chiral flavour space for the explicit chiral flavour symmetry breaking. Our physical interpretation is such that by definition only the axial generators are broken by the mass term thus defining the residual vector symmetry. With Wilson quarks at non-zero $\alpha$ there is an additional breaking of flavour symmetry by the Wilson term, which is expected to disappear in the continuum limit, just like chiral symmetry is restored with standard Wilson quarks. In order to define the continuum limit properly one must make sure that cutoff effects are a smooth function of $\beta = 6/g_0^2$. In general this can be achieved by taking the continuum limit at constant physical conditions. For instance one may keep $m_\pi/F_\pi$ constant as $\beta$ is varied. However, in tmQCD this observable is a function of two mass parameters, or, equivalently of one mass parameter and the twist angle. It is crucial that the twist angle is kept constant as
the continuum limit is taken, since the twist angle labels different lattice regularisations of two-flavour QCD. In particular, if $\alpha$ is changed from one $\beta$-value to the next, there is no reason to expect a smooth continuum approach and a continuum extrapolation may become impossible.

5. A few applications of tmQCD

The relations between tmQCD and standard QCD correlation functions can be used to by-pass certain lattice renormalization problems of standard Wilson quarks (cf. sect. 3). As the different operators of a continuum chiral multiplet are not necessarily related by lattice symmetries, their renormalisation properties can be very different. Moreover, the renormalisation properties do not change in the presence of (twisted or non-twisted) mass terms except when power divergences are present. Excluding these cases it is thus sufficient to renormalise a given composite field in the chiral limit where the actions of tmQCD and standard Wilson quarks coincide. One may then choose the operator with the best renormalisation properties that can be related to the desired standard QCD operator by the dictionary established earlier. Moreover, it may not even be necessary to match the operators directly. In principle, it is enough to match the desired correlation function up to cutoff effects. Perhaps these remarks become clearer by going through a few examples:

5.1. Computation of $F_\pi$

Both the pion mass $m_\pi$ and the pion decay constant $F_\pi$ can be obtained from the long distance behaviour of the 2-point function

$$\left\langle (A_R)_0^1(x)(P_R)^1(y) \right\rangle_{(M_R,0)} = \cos(\alpha) \left\langle (A_R)_0^1(x)(P_R)^1(y) \right\rangle_{(M_R,\alpha)} + \sin(\alpha) \left\langle \tilde{V}_0^2(x)(P_R)^1(y) \right\rangle_{(M_R,\alpha)}. \quad (35)$$

The problem with the standard Wilson computation on the l.h.s. is that the axial current requires a non-trivial renormalisation, which needs to be determined from Ward identities, as done e.g. in $^6$. On the other hand the vector current $\tilde{V}_\mu^a$ is protected against such a rescaling since it is conserved at $\mu_q = 0$. At $\alpha = \pi/2$ the axial current is mapped to the vector current and one may thus avoid the current renormalisation by computing the vector correlation function in tmQCD. It is in fact not necessary to set $\alpha = \pi/2$;
when inverting the relation (35),
\[ \langle \tilde{V}_0^2(x)(P_R)_{1}^y \rangle_{(M_R,\alpha)} = \cos(\alpha) \langle \tilde{V}_0^2(x)(P_R)_{1}^y \rangle_{(M_R,0)} + \sin(\alpha) \langle (A_R)^0_{1}(x)(P_R)_{1}^y \rangle_{(M_R,0)} . \] (36)

one notices that the first term on the r.h.s violates both parity and flavour symmetry of standard QCD. On the lattice this correlation function therefore contributes at most an \( O(a) \) effect. One may thus obtain \( F_\pi \) at values \( \alpha \neq \pi/2 \) by computing the l.h.s of this equation. Finally, it should be mentioned that the exact PCVC lattice relation,
\[ \partial_\mu \tilde{V}_a^\mu = -2\mu_2 \varepsilon^{ab} P^b, \] (37)

may be used to replace the vector current by the axial density. Summing over \( x \), translation invariance eliminates the spatial part of the divergence, and the time derivative reduces to a multiplication by \( m_\pi \) at large time separations\(^{17}\). The results of a quenched computation along these lines\(^{18,19}\) are shown in figures 2 and 5.

5.2. Direct determination of the chiral condensate

A computation of the chiral condensate from the local scalar density has never been performed with Wilson quarks, due to the cubic divergence (9) which persists in the chiral limit. In tmQCD the rôle of the scalar density is played by the axial density, i.e. one expects the relation
\[ \langle (P_R)^3(x) \rangle_{(M_R,\alpha)} = \cos(\alpha) \langle (P_R)^3(x) \rangle_{(M_R,0)} - \frac{i}{2} \sin(\alpha) \langle (S_R)^0(x) \rangle_{(M_R,0)} \] (38)

Again, the first term on the r.h.s. vanishes up to \( O(a) \) due to parity, so that the computation of the l.h.s. yields the chiral condensate up to the factor \((-i/2)\sin(\alpha)\). This is advantageous as the renormalised axial density is of the form,
\[ (P_R)^3 = Z_P \left( P^3 + \mu_2 c_2 \ a^{-2} \right), \] (39)

i.e. the power divergence vanishes for \( \mu_2 = 0 \). Still, in order to determine the condensate one needs to perform first the infinite volume limit followed by the \( \mu_2 = 0, m_0 = m_{cr} \) limits (at fixed \( \alpha \)) and the continuum limit, which remains a rather delicate task. In particular, the chiral limit is complicated by the fact that the uncertainty in \( \sin(\alpha) \) increases as the quark mass is decreased, due to the intrinsic \( O(a) \) ambiguity of \( m_{cr} \). In practice this means that one has to extrapolate to the chiral limit from some distance, but this is anyway required for finite volume effects to remain small.
5.3. The computation of $B_K$

Four-quark operators provide an interesting playground for mappings between tmQCD and standard QCD. We start with the $B_K$ parameter which is defined in QCD with dynamical $u,d,s$ quarks by,

$$\langle \bar{K}^0 | O_{(V-A)(V-A)}^{\Delta S=2} | K^0 \rangle = \frac{8}{3} F_K^2 m_K^2 B_K. \quad (40)$$

The local operator

$$O_{(V-A)(V-A)}^{\Delta S=2} = \sum_{\mu} \bar{s} \gamma_{\mu} (1 - \gamma_5) d^2,$$  \quad (41)

is the effective local interaction induced by integrating out the massive gauge bosons and $t,b$- and $c$-quarks in the Standard Model. The transition between the pseudoscalar states $K^0$ and $\bar{K}^0$ does not change parity. Therefore, only the parity-even part in the effective operator,

$$O_{(V-A)(V-A)} = O_{VV+AA}^{\text{parity-even}} - O_{VA+AV}^{\text{parity-odd}}, \quad (42)$$
contributes to $B_K$. With Wilson type quarks, the operators $O_{VV+AA}$ and $O_{VA+AV}$ are renormalised as follows

$$ (O_{VV+AA})_R = Z_{VV+AA} \left\{ O_{VV+AA} + \sum_{i=1}^{4} z_i \, O_{d=6}^i \right\} , \quad (43) $$

$$ (O_{VA+AV})_R = Z_{VA+AV} \, O_{VA+AV} . \quad (44) $$

While the parity-even component mixes with four other operators of dimension 6, the parity-odd component only requires multiplicative renormalisation, due to CP and flavour exchange symmetries. This raises the question if one can by-pass the mixing problem by exchanging the roles of both operators through the introduction of twisted mass terms. This is indeed possible, but one first needs to introduce the strange quark. The simplest possibility consists in adding a standard $s$-quark to a twisted quark doublet $\psi$ of the light up and down quarks, which are thus taken to be degenerate. The corresponding continuum Lagrangian is given by

$$ L = \bar{\psi} \left( \frac{D}{i} + m + i \mu_q \gamma^5 \tau^3 \right) \psi + \bar{s} \left( \frac{D}{i} + m_s \right) s , \quad (45) $$

and, passing to the physical basis of primed fields, one finds

$$ O'_{VV+AA} = \cos(\alpha) O_{VV+AA} - i \sin(\alpha) O_{VA+AV} = -i O_{VA+AV} \quad (\alpha = \pi/2). \quad (46) $$

At full twist, we thus get a direct mapping between both operators, i.e. $O_{VA+AV}$ in twisted mass QCD at $\pi/2$ is interpreted as $O_{VV+AA}$ in standard QCD. A second possibility consists in exchanging the roles of up and strange quark, i.e. one considers a twisted doublet of strange and down quarks and a standard $u$-quark. In this case one finds

$$ O'_{VV+AA} = \cos(2\alpha) O_{VV+AA} - i \sin(2\alpha) O_{VA+AV} = -i O_{VA+AV} \quad (\alpha = \pi/4) , \quad (47) $$

i.e. the same mapping is obtained, but with the twist angle $\alpha = \pi/4$. Several comments are in order: while both options, referred to as $\pi/2$ and $\pi/4$ scenarios respectively, are possible, the second one is clearly more remote from reality, as it assumes mass degenerate down and strange quarks. However, this is precisely the limit in which most lattice calculations to date have been performed. The justification rests on chiral perturbation theory where a a weak dependence upon the strange-down mass difference is predicted. Moreover, in the quenched approximation, any deviation from the degenerate case leads to an unphysical logarithmic quark mass dependence.
5.3.1. Renormalisation of $O_{VA+AV}$

Whatever the chosen strategy, the operator which requires renormalisation is $O_{VA+AV}$. The renormalisation is multiplicative, and the general strategy of \cite{23} can be applied. The scale evolution of the operator in a few Schrödinger functional schemes has been traced in the quenched approximation over a wide range of scales (for first results with $N_f = 2$ sea quarks cf. \cite{24}). The result is shown in figure 3. It thus remains to calculate the bare matrix element for $B_K$ at various values of $\beta$, and, after multiplication with the $Z$-factor at the low energy scale, perform the continuum limit extrapolation. In the continuum limit one may then use the known scale evolution to reach the truly perturbative regime where contact is made with the perturbative renormalisation schemes of the continuum.

![Graph showing scale evolution of $B_K$](image)

Figure 3. The data points show the non-perturbatively computed scale evolution of $B_K$ in the SF scheme. Also shown are two perturbative approximations.
5.3.2. Results for $B_K$ in the quenched approximation

Both scenarios have been implemented in the quenched approximation with lattice spacings $a = 0.05 - 0.1$ fm and lattice sizes up to $L/a = 32$. If one sticks to mass degenerate down and strange quarks the $\pi/2$ scenario requires some chiral extrapolation, due to the problem with unphysical zero modes (recall that the $s$-quark remains untwisted). In the $\pi/4$ scenario the zero mode problem is eliminated and the kaon mass can be reached by interpolation, provided the finite volume effects are small enough. This is the case with all lattice spacings except the finest one, where some extrapolation is required. A combined continuum extrapolation to both data sets, linear in $a$, leaving out the data at the coarsest lattice spacing led to the result $\hat{B}_K = 0.789(46)$, where $\hat{B}_K$ denotes the renormalisation group invariant $B$-parameter. Unfortunately, the twist angle at $\beta = 6.1$ had not been tuned precisely enough, a fact that was only noticed after publication of $25$. A new analysis indicates that higher than linear lattice artefacts are still significant at $\beta = 6.1$. As the data set is not sufficient to fit to both $a$ and $a^2$ terms, it was decided to discard the data at $\beta = 6.1$, too, with the result $28$

$$\hat{B}_K = 0.735(71) \iff \hat{B}_K^{\text{MS}}(2 \text{ GeV}) = 0.534(52),$$

which is compatible with the earlier result, albeit with a larger uncertainty. In conclusion, the quenched result for $B_K$ has a total error of almost 10 percent, which includes all systematic effects (renormalisation, chiral interior or extrapolations, continuum extrapolation) except quenching and the fact that the valence quarks are mass degenerate. However a variation of the mass difference up to $(M_s - M_d)/(M_s + M_d) \approx 0.5$ did not show sizeable effects. While the error could still be improved by including data at a finer lattice spacing it seems fair to say that further progress requires the inclusion of sea quark effects.

5.4. Further applications

Twisted mass QCD does not provide a general recipe for by-passing the lattice specific renormalisation problems of Wilson quarks. Rather, one needs to discuss on a case by case basis whether it can be advantageous to use some variant of tmQCD. For further applications to four-quark operators and $K \to \pi$ transitions I refer the reader to $26,27$. While the first reference insists on an equal treatment of sea and valence quarks, the second paper explores a mixed action approach, where the valence quarks are chirally
twisted individually, independently of the sea quark action. This yields a much greater flexibility and allows for a complete elimination of lattice specific mixings and subtractions, even including O(a) improvement. Finally, similar considerations apply to QCD with static b-quarks, where the mixing of four-quark operators is considerably simplified by twisting the light quarks (see 28 for a recent review and further references).

6. O(a) improvement and tmQCD
Given that the quenched approximation is currently being overcome, and the zero mode problem for algorithms can be alleviated, there remain essentially two arguments in favour of tmQCD as opposed to standard or O(a) improved Wilson quarks: the first consists in the possibility to by-

Figure 4. Quenched lattice data for both scenarios, $\alpha = \pi/2$ and $\alpha = \pi/4$. Also shown is the combined continuum extrapolation, leaving out the data at the two coarsest lattice spacings.
pass renormalisation problems, as explained in the preceding section. The second, is the property of “automatic O(a) improvement” at maximal twist (i.e. $\alpha = \pi/2$), as first observed by Frezzotti and Rossi 4. I will explain this point more in detail below, after a brief reminder of the situation with standard Wilson quarks.

6.1. \textit{O(a) improvement of Wilson quarks}

In lattice QCD with Wilson quarks, results are typically affected by O(a) lattice effects, which is to be contrasted with staggered or Ginsparg-Wilson quarks where the leading cutoff effects are quadratic in $a$. As illustrated by the $B_K$ determination described above, linear lattice artefacts render continuum extrapolations more difficult, and it would be nice to get rid of them altogether. This is possible by introducing O(a) counterterms to the action and the composite operators such that O(a) effects are cancelled in on-shell quantities. The basic idea goes back to Symanzik 29, while the restriction to on-shell quantities in gauge theories has been first advocated by Lüscher and Weisz 30. When applied to Wilson quarks 31, it turns out that O(a) improvement of the spectrum (particle masses and energies) can be achieved by adding a single counterterm to the action, the so-called Sheikholeslami-Wohlert (SW) or clover term, $i \bar{\psi} \sigma_{\mu\nu} F_{\mu\nu} \psi$, where $F_{\mu\nu}$ is the gluon field tensor $^e$. This term is of dimension five and therefore comes with an explicit factor $a$ when included in the lattice action density.

While O(a) improvement of the spectral quantities is quite economical, one is often interested in matrix elements of composite operators, and each operator comes with its own set of O(a) counterterms, all of which have to be tuned in order to cancel the linear lattice artefacts. While this may still be possible for quark bilinear operators, the counterterms quickly proliferate in the case of 4-quark operators, and O(a) improvement becomes completely impractical if the quarks are taken to be mass non-degenerate (cf. 32).

6.2. \textit{Automatic O(a) improvement of tmQCD in a finite volume}

The Symanzik effective theory can also be applied to tmQCD and a list of O(a) counterterms for the action and a few quark bilinear operators can be found in 3. The observation in 4 is, that at maximal twist, all the O(a) coun-

$^e$On the lattice the field tensor is usually discretised using four plaquette terms in the $(\mu, \nu)$-plane whence the name “clover term”.
terms become irrelevant in the sense that they can at most contribute at $O(a^2)$. The argument for automatic $O(a)$ improvement can be made such that it only relies on Symanzik's effective continuum theory. To simplify the discussion, let us first assume that the space-time volume is finite, so that spontaneous symmetry breaking is excluded and all observables are analytic in the quark mass parameters. We furthermore assume that we have tuned some PCAC current quark mass $m_{\text{PCAC}} = 0$, i.e. the renormalized standard mass parameter vanishes up to $O(a)$ effects. Then Symanzik's effective continuum action is given by

$$S_{\text{eff}} = S_0 + a S_1 + O(a^2), \quad S_0 = \int d^4 x \, \bar{\psi} (\not{D} + i \mu_\gamma \gamma^5 \tau^3) \psi,$$

where $S_0$ is the maximally twisted tmQCD continuum action. $S_1$ is given by

$$S_1 = \int d^4 x \, \{ c \, i \bar{\psi} \sigma_{\mu\nu} F_{\mu\nu} \psi + b \mu^2 \bar{\psi} \psi + \ldots \},$$

where the dots stand for further operators of dimension 5 (possibly including explicit mass factors), which share the symmetries of the lattice action. The reason why I omitted them here is that they can be eliminated by the equations of motion. Furthermore, the second operator can be absorbed in an $O(a)$ shift of the standard quark mass parameter, so that one is really left with the SW term as the only relevant operator for on-shell improvement.

Renormalised (connected) lattice correlation functions can be analysed in the effective theory,

$$\langle O \rangle = \langle O \rangle_{\text{cont}} - a \langle S_1 O \rangle_{\text{cont}} + a \langle \delta O \rangle_{\text{cont}} + O(a^2),$$

where the cutoff dependence is explicit. We are here only interested in the leading cutoff effects at $O(a)$. To this order there are two contributions, first the insertion of the $O(a)$ part of the effective action $S_1$, and second the field specific counterterms $\delta O$. For example, with the choice

$$O = V^1_\mu(x) P^2(y),$$

one finds the counterterm,

$$\delta O = \{ c_v i \partial_\nu T^{1}_{\mu\nu}(x) + \tilde{b}_v \mu_q A^{2}_\mu(x) \} P^2(y) + \ldots,$$

where the dots stand for further terms which vanish by the equations of motion. It should be emphasised that the $O(a)$ (and higher) corrections in the effective action are only treated as insertions, i.e. the expectation values $\langle \cdot \rangle_{\text{cont}}$ are taken with respect to the continuum action $S_0$. In writing down
the effective Symanzik theory there is thus an implicit assumption made, namely that one is working in the regime of continuum QCD where cutoff effects only appear as asymptotically small corrections. This assumption may certainly be wrong in some regions of parameter space, and particular care has to be taken in the presence of phase transitions.

To proceed I introduce the $\gamma_5 \tau^1$-transformation,

$$\psi \rightarrow i \gamma_5 \tau^1 \psi, \quad \bar{\psi} \rightarrow \bar{\psi} i \gamma_5 \tau^1,$$  \hspace{1cm} (54)

which is part of the vector symmetry of two-flavour QCD. Hence $S_0$ is invariant, but this is not the case for $S_1$, i.e. one finds

$$S_0 \rightarrow S_0, \quad S_1 \rightarrow -S_1.$$  \hspace{1cm} (55)

For gauge invariant fields the transformation (54) squares to the identity, so that one may define an associated parity. For fields $O$ with a definite $\gamma_5 \tau^1$-parity one then finds,

$$O \rightarrow \pm O \Rightarrow \delta O \rightarrow \mp \delta O.$$  \hspace{1cm} (56)

By applying the $\gamma_5 \tau^1$ transformation to the integration variables in the functional integral, one may derive identities between correlation functions, due to the invariance of the continuum action and functional measure. In particular, if we choose a $\gamma_5 \tau^1$-even field $O$, we find for the correlation functions at $O(a)$

$$\langle S_1 O \rangle^\text{cont} = -\langle S_1 O \rangle^\text{cont} = 0,$$
$$\langle \delta O \rangle^\text{cont} = -\langle \delta O \rangle^\text{cont} = 0,$$  \hspace{1cm} (57)

and therefore

$$\langle O \rangle = \langle O \rangle^\text{cont} + O(a^2).$$  \hspace{1cm} (58)

For a $\gamma_5 \tau^1$-odd $O$, one obtains

$$\langle O \rangle^\text{cont} = -\langle O \rangle^\text{cont} = 0,$$
$$\langle S_1 O \rangle^\text{cont} = \langle S_1 O \rangle^\text{cont},$$
$$\langle \delta O \rangle^\text{cont} = \langle \delta O \rangle^\text{cont},$$  \hspace{1cm} (59)

which implies

$$\langle O \rangle = -a \langle S_1 O \rangle^\text{cont} + a \langle \delta O \rangle^\text{cont} + O(a^2).$$  \hspace{1cm} (60)

We may thus conclude that, at least in a small finite volume lattice correlation functions of $\gamma_5 \tau^1$-even fields are automatically $O(a)$ improved, while those of $\gamma_5 \tau^1$-odd fields vanish up to $O(a)$ terms. As a corollary, one may
state that standard Wilson quarks in a finite volume are automatically \( O(a) \) improved in the chiral limit. Although this is not the most interesting regime of QCD, it is somewhat surprising that this fact had not been noticed for more than 2 decades! To conclude this section note that in terms of the physical basis, (54) corresponds to the discrete flavour transformation,

\[
\psi' \rightarrow -i\tau^2\psi', \quad \bar{\psi}' \rightarrow \bar{\psi}'i\tau^2.
\] (61)

A very similar argument based on parity transformations has been given by Shindler in 5. In 35 a systematic analysis of the \( \gamma_5\tau^1 \) symmetry (called \( T_1 \) in this paper) can be found, showing that not only \( O(a) \) but all odd powers of \( a \) vanish in \( \gamma_5\tau^1 \)-even correlators. This is not surprising, as this is implicit in the earlier analysis in 4, where the same conclusion was drawn.

6.2.1. Uncertainty of the chiral limit

If \( O(a) \) improvement is automatic one might think that it should be possible to determine the critical mass \( m_{cr} \) up to an intrinsic \( O(a^2) \) uncertainty. This is not so, as I will now explain. The critical mass can be determined by tuning some PCAC mass to zero, and there is no obstacle for doing this in a finite volume. Now, the PCAC relation involves the axial current and density, \( A_{\mu}^a \) and \( P^a \), which have opposite \( \gamma_5\tau^1 \)-parities. According to the preceding discussion this means, for the first flavour components and with a \( \gamma_5\tau^1 \)-even source field \( O_{\text{even}} \),

\[
\langle \partial_\mu A_{\mu}^1(x)O_{\text{even}} \rangle = 2m_{\text{PCAC}}\underbrace{\langle P^1(x)O_{\text{even}} \rangle}_{O(a)} = O(a^2).
\] (62)

The l.h.s. being \( \gamma_5\tau^1 \)-even must vanish up to \( O(a^2) \), provided maximal twist is realised at least up to cutoff effects, i.e. \( m_R = O(a) \). This implies that the PCAC mass is of \( O(a) \), too, multiplying a correlation function which is \( \gamma_5\tau^1 \)-odd and therefore of \( O(a) \). Thus no contradiction arises, the \( O(a^2) \) of the l.h.s. is matched on the r.h.s. by two factors of \( O(a) \).

Another way to understand that an \( O(a) \) shift in the critical mass does not ruin \( O(a) \) improvement is to treat such a shift as an insertion of the standard mass operator \( \bar{\psi}\psi \) into correlation functions. This operator is \( \gamma_5\tau^1 \)-odd so that its insertion into a \( \gamma_5\tau^1 \)-even correlator produces an \( O(a) \) effect, which together with the \( O(a) \) mass shift yields an \( O(a^2) \) effect.
6.3. Automatic $O(a)$ improvement in infinite volume

When the infinite volume limit is taken, the basic difference is the presence of spontaneous symmetry breaking and the appearance of non-analyticities in the mass parameters near the chiral limit. As discussed earlier, twisted mass QCD is a valid regularisation of two-flavour QCD provided the continuum limit is taken at fixed twist angle. To maintain maximal twist, i.e. $\alpha = \pi/2$ one needs to tune the standard quark mass to $m_{cr}$, which has an intrinsic $O(a)$ ambiguity. As long as the twisted mass is much larger than the typical $O(a)$ spread of $m_{cr}$, the twist angle may be considered well-defined, and the continuum limit is reached with $O(a^2)$ corrections. However, in practice one is interested in varying the quark mass at fixed cutoff, rather than studying the quark mass dependence only in the continuum limit. Approaching the chiral limit at fixed $a$ by lowering the twisted mass one enters the regime where the twisted mass parameter becomes comparable to the $O(a)$ ambiguity of $m_{cr}$. One may debate at this point whether the relevant comparison is with the uncertainty of $m_{cr}$ itself or rather with the size of typical $O(a^2)$ effects in correlation functions generated by this uncertainty. In any case one reaches a point where the control over the twist angle is lost. When delivering my Nara lectures I interpreted this fact as a breakdown of the effective Symanzik theory. This is perhaps too rigid an interpretation. Rather one could say that for every definition of $m_{cr}$, an effective twist angle is formed by the dynamics of the system, which may be far from the maximal twist one would like to maintain. Moreover, without further input is is impossible to know the effective twist angle for a given definition of $m_{cr}$. This is a disaster, as the whole interpretation of the theory rests on the twist angle, and a change in the effective twist angle (which remains unnoticed!) might strongly affect some correlators even at $O(1)$! Fortunately this problem occurs close to the chiral limit, and thus in a region of parameter space where Chiral Perturbation Theory ($\chi$PT) is expected to describe the dynamics in terms of pion physics. In particular, $\chi$PT is able to identify definitions of $m_{cr}$ in terms of pionic observables, which lead to an effective twist angle of $\alpha = \pi/2$, so that the Symanzik effective theory for maximally twisted mass QCD remains applicable in this region. For instance, this should be the case if one requires parity or flavour symmetry restauration, e.g. by imposing that a $\gamma_5\tau^1$-odd pion correlation function vanishes. Note that the vanishing of the PCAC mass for a pion correlation function is a special case of such a condition. On the other hand, according to $^{37,35}$ the condition of vanishing pion mass
(calculated in the untwisted theory) does indeed lead to a $O(1)$ variation of the effective twist angle. However, apart from larger cutoff effects of $O(a^2)$ this does not (yet?) seem to be a major problem in $^{19}$, cf. figure 5. In any case, as the spontaneous symmetry breaking is closely related to the dynamics of pions, it seems that no statement can be made about generic definitions of $m_{cr}$ in a small volume, either from axial current conservation, or from parity or flavour symmetry restauration.

![Figure 5](attachment:figure5.png)

Figure 5. The continuum approach of $F_\pi$ in quenched tmQCD for various pion masses vs. $a^2/r_0^2$.

7. Consequences of Parity and Flavour breaking

The exact symmetries of lattice QCD with standard Wilson quarks include parity and flavour symmetry which are used to classify the hadron spectrum. This is very convenient in any hadron analysis: even at fixed lattice spacing, the excited states which may occur in a given channel can be read from the Particle Data Book, with the exception of states with higher spin and/or angular momentum where the correspondence is spoilt by the lack
of rotational symmetry on the lattice.

The situation is different in tmQCD since both parity and flavour symmetry are broken by the Wilson term. As a consequence, the classification in isospin multiplets fails by terms of $O(a)$, or $O(a^2)$ if $O(a)$ improvement is at work. For instance, the neutral pion is not mass degenerate with the charged pions, or the nucleon $\Delta$-resonances no longer form an exact isospin multiplet. Various simulations of quenched tmQCD have confirmed these expectations, and point to a restoration of flavour symmetry in the continuum limit\(^{38,39,40}\), although the expected rate $\propto a^2$ for maximally twisted mass QCD has not in all cases been demonstrated convincingly.

However, the splittings of isospin multiplets by cutoff effects are not the most serious drawback of parity and flavour symmetry breaking. In the spectral analysis of a hadronic two-point function all excited states with the same lattice quantum numbers may contribute. Even though the states violating continuum symmetries are multiplied by coefficients proportional to $a$, these states need to be taken into account when working at fixed lattice spacing. Particularly annoying is the neutral pion, which shares all the lattice quantum numbers with the vacuum. One may thus add a neutral pion to any state without changing its lattice quantum numbers. The presence of additional relatively light states may require a multistate analysis just to identify and subtract states which are a pure lattice artefact. Moreover, correlation functions involving the light pion require the evaluation of disconnected diagrams. However, it should be emphasised that these problems are purely technical; conceptually tmQCD is on a very solid basis, and in contrast to staggered fermions there is no mixing between flavour and spin degrees of freedom.

### 7.1. Non-degenerate quarks and additional flavours

Twisted mass QCD was originally formulated for a single doublet of mass degenerate flavours. This can easily be generalised to include more mass degenerate doublets. However, such a spectrum is quite unrealistic unless a non-degeneracy can be introduced within a doublet. Moreover, this non-degeneracy should not cause too much damage to all the nice properties of tmQCD. In particular, one needs to maintain the reality and positivity of the quark determinant, if such an action is to be used for simulations of full tmQCD. This is indeed possible, by introducing a mass splitting term as follows\(^ {41}\),

$$
\mathcal{L} = \bar{\psi} ( \slashed{D} + m + i \mu \gamma_5 \tau^3 + \delta m \tau^1 ) \psi,
$$

(63)
where $\delta_m$ is the mass splitting parameter. The mass spectrum is easily obtained by going to the physical basis and diagonalising the mass matrix. Its eigenvalues are then found to be $M_\pm = \sqrt{m^2 + \mu^2} \pm \delta_m$. Translating this continuum situation to Wilson quarks in the obvious way, one first notices that the determinant of the twisted Wilson-Dirac operator must be real due to the conjugation property,

$$\gamma_5 \tau_1 \left( DW + m_0 + i\mu q \gamma_5 \tau_3 + \delta_m \tau_1 \right) \gamma_5 \tau_1 \right) = \left( DW + m_0 + i\mu q \gamma_5 \tau_3 + \delta_m \tau_1 \right) \tau_1 \right).$$

Furthermore, the flavour structure of the determinant can again be reduced analytically, with the result,

$$\det(DW + m_0 + i\mu q \gamma_5 \tau_3 + \delta_m \tau_1) = \det(Q^2 + \delta_m [\gamma_5, Q] + \mu^2 - \delta^2_m),$$

and this determinant is non-zero provided $\mu^2 > \delta^2_m$. The positivity of the determinant at $\delta_m = 0$ and continuity in $\delta_m$ then imply positivity of this determinant for non-zero $\delta_m$.

The mass splitting parameter is renormalised multiplicatively $\delta_{m,R} = Z_S^{-1} \delta_m$, where $Z_S$ is the renormalisation constant of the non-singlet scalar density. As the positivity of the determinant follows from a condition on the bare parameters $\mu_q$ and $\delta_m$, the corresponding condition in terms of the renormalised parameters involves a ratio of renormalisation constants, i.e. $\delta_{m,R} < (Z_P/Z_S)\mu_R$. The value of $Z_P/Z_S$ depends on details of the regularization, so that one cannot make a general statement about the ensuing limitations (if any). However, it is remarkable that one may use this action to perform numerical simulations with two non-degenerate light quark flavours, as needed for instance to study small isospin breaking effects. If used for strange and charm quarks $^{42,43}$, however, one potentially has to deal with a fine tuning problem for the strange quark mass: for instance, assuming $m_s = 100$ MeV and $m_c = 1300$ MeV, these values are obtained as $(700 \pm 600)$ MeV. Finally, it should be said that the presence of the additional flavour non-diagonal breaking term renders the relationship to standard QCD more complicated, and the flavour structure needs to be dealt with explicitly in numerical calculations of quark propagators.

8. A chiral twist to the QCD Schrödinger functional

In order to solve scale dependent renormalisation problems the introduction of an intermediate renormalisation scheme based on the Schrödinger
functional (SF scheme) is an attractive possibility. Here I start by summarising its basic features in order to prepare the discussion of possible improvements.

8.1. The QCD Schrödinger functional

The QCD Schrödinger functional\textsuperscript{44,45}(SF) is the functional integral for QCD where the Euclidean space-time manifold is taken to be a hyper cylinder. The quantum fields are periodic in space, and Dirichlet conditions are imposed at (Euclidean) times $x_0 = 0$ and $x_0 = T$.

$$P_+ \psi(x) \mid_{x_0=0} = \rho, \quad P_- \psi(x) \mid_{x_0=T} = \rho'$$

$$\bar{\psi}(x) P_- \mid_{x_0=0} = \bar{\rho}, \quad \bar{\psi}(x) P_+ \mid_{x_0=T} = \bar{\rho}$$

$$A_k(x) \mid_{x_0=0} = C_k, \quad A_k(x) \mid_{x_0=T} = C'_k, \quad k = 1, 2, 3$$

(66)

with the projectors $P_\pm = \frac{1}{2}(1 \pm \gamma_0)$. Correlation functions are then defined as usual,

$$\langle O \rangle = \left\{ Z^{-1} \int_{\text{fields}} O \, e^{-S} \right\}_{\rho=\rho'=0; \bar{\rho} = \bar{\rho}'=0}.$$  (67)

$O$ denotes some gauge invariant functional of the fields, possibly including the quark and antiquark boundary fields $\zeta$ and $\bar{\zeta}$, which are obtained by taking derivatives with respect to the quark boundary fields, viz.

$$\zeta(x) \equiv P_- \zeta(x) = \frac{\delta}{\delta \rho(x)}, \quad \bar{\zeta}(x) \equiv \bar{\zeta}(x) P_- = -\frac{\delta}{\delta \rho(x)}.$$  (68)

The name “Schrödinger functional” derives from the fact that such wave functionals arise naturally in the Schrödinger representation of Quantum Field Theory\textsuperscript{46}, and the SF provides an example of a Quantum Field Theory defined on a manifold with a boundary.

Using correlation functions derived from the Schrödinger functional, it is possible to define renormalised QCD parameters (the strong coupling and the quark masses), as well as renormalised composite operators (e.g. four-quark operators). Such renormalization schemes based on the Schrödinger functional (SF schemes) are attractive for the following reasons:

- The finite volume is part of the scheme definition, i.e. all dimensionful quantities such as Euclidean time extent $T$, or boundary field parameters are scaled proportionally to $L$, the linear extent of the volume. As a consequence $L$ remains the only scale in the system and can be identified with the renormalization scale by setting
\( \mu = L^{-1} \). Running parameters and operators then run with the size of the space-time volume, and one may apply recursive finite size techniques to bridge large scale differences (cf. subsect. 5.3.1)

- SF schemes are made quark mass independent by imposing the renormalisation conditions in the chiral limit. Fortunately, the SF boundary conditions introduce a gap in the spectrum of the Dirac operator, which persists as the quark mass is taken to zero. This means that numerical simulations can be performed in the chiral limit, and no chiral extrapolation is needed to evaluate the renormalisation conditions.
- SF schemes are gauge invariant, no gauge fixing is needed.
- Perturbation theory up to two loops is still feasible, due to the existence of a unique absolute minimum of the action\(^{44}\). This is to be contrasted with the situation on a hyper torus where perturbation theory becomes very intricate already at the one-loop level.
- A further technical advantage consists in the possibility to use correlators involving zero momentum boundary quark and anti-quark fields. This is convenient in perturbation theory, and it leads to good numerical signals and reduced cutoff effects as compared to gauge invariant correlators in a periodic setting.

All these nice properties come with a price: first of all, the presence of the boundary means that even the pure gauge theory suffers from \( O(a) \) cutoff effects, caused by effective local operators of dimension 4, such as \( \text{tr}\{F_{ik}F_{jk}\} \) and \( \text{tr}\{F_{ik}F_{ik}\} \), integrated over the boundary. When the quarks are included, there is even a dimension 3 operator, which can be absorbed in a multiplicative rescaling of the quark and antiquark boundary fields\(^{47}\). At order \( a \), one expects dimension 4 operators like \( \bar{\psi}\gamma_0 D_0 \psi \) and \( \bar{\psi}\gamma_k D_k \psi \) to contribute additional \( O(a) \) effects\(^6\). It is important to note that these cutoff effects are, unlike the \( O(a) \) bulk effects of Wilson quarks, not due to the breaking of a continuum symmetry by the regularisation. Rather, such terms are to be expected with any regularisation of the Schrödinger functional. One may, however, write down a complete basis of \( O(a) \) counterterms which contribute to a given observable. After reduction via the equations of motion, one typically ends up with 2-3 \( O(a) \) boundary counterterms. In practice it is then possible to monitor the size of the boundary \( O(a) \) effects by varying the coefficients. Perturbative results for these coefficients are often known to one-loop or even two-loop order\(^{48}\), and a non-perturbative determination may be conceivable. In summary, with some
extra work, the $O(a)$ boundary effects can be controlled and eventually eliminated. This is important, as otherwise the SF renormalisation procedure risks to introduce $O(a)$ effects even in $O(a)$ improved regularisations such as tmQCD at maximal twist or lattice QCD with Ginsparg-Wilson quarks.

8.2. Decoupling of heavy quarks in SF schemes

Quark mass independent schemes are very convenient to study the scale evolution for a theory with fixed quark flavour content. However, it also means that the decoupling of heavy quarks is not automatic, and one needs to match theories with different numbers of active flavours over quark thresholds. This is routinely done in perturbation theory, but it is not obvious that perturbation theory is adequate e.g. for matching the $N_f = 4$ and $N_f = 3$ effective theories over the charm quark threshold. One possibility to study decoupling consists in introducing a quark mass dependent SF scheme which would allow to study the non-perturbative evolution over the quark threshold until the heavy quark has decoupled. To define a mass dependent SF scheme it suffices to impose the renormalisation conditions at finite quark masses. Unfortunately, it turns out that the decoupling of a heavy quark in such a scheme is only linear in the inverse quark mass rather than quadratic. If the quark decouples very slowly, this means that it has to be kept longer in the evolution as an active degree of freedom, which could mean that widely different scales have to be accomodated on the same lattice.

An example from perturbation theory\textsuperscript{49,50} is given in figure 6. It shows the one-loop $\beta$-function of the running coupling in the SF scheme as a function of $z = mL$, where $m$ is some renormalised quark mass (its precise definition is not required to one-loop order). As $z = mL$ is varied from 0 to infinity, one expects to see a smoothed out step function going from $-1$ to 0 around the threshold $z = 1$. The solid and dotted curves (from 2 different SF schemes) do indeed show this behaviour, but the decoupling is rather slow compared to the MOM scheme\textsuperscript{51} (dashed line).

To understand this behaviour I propose a closer look at the Dirac operator for free quarks and its spectrum in the continuum limit.
8.2.1. Free quarks with SF boundary conditions

Let us consider a free quark $\psi$ in the continuum with homogeneous SF boundary conditions,

$$P_+ \psi(x) \mid_{x_0=0} = 0, \quad P_- \psi(x) \mid_{x_0=T} = 0.$$  \hspace{1cm} (69)

Then $\gamma_5(\not{\partial} + m)$ is a hermitian operator with smooth eigenfunctions and no zero modes \(45\). Evaluating the eigenvalue equation for any of its eigenfunctions $\varphi$ at the boundaries one finds,

$$P_+ \gamma_5(\not{\partial} + m) \varphi \mid_{x_0=0} = 0 \quad \Rightarrow \quad (\partial_0 - m)P_- \varphi \mid_{x_0=0} = 0,$$

$$P_- \gamma_5(\not{\partial} + m) \varphi \mid_{x_0=T} = 0 \quad \Rightarrow \quad (\partial_0 + m)P_+ \varphi \mid_{x_0=T} = 0. \hspace{1cm} (70)$$

The complementary components thus satisfy Neumann conditions modified by the mass term $m$. The eigenvalues $\lambda$ are of the form $\lambda = \ldots$
\[ \pm \sqrt{p_0^2 + p^2 + m^2}, \]
where \( p_0 \) is determined as non-vanishing solution of \( \tan(p_0 T) = -p_0/m \). It is obvious from this equation that \( p_0 \) and thus \( \lambda \) are not symmetric under \( m \to -m \). This is generic and can be understood as a consequence of chiral symmetry breaking by the boundary conditions. As a result one expects, for any observable in the SF, the asymptotic small mass behaviour \( \propto m \) (rather than \( m^2 \)), and similarly for heavy quarks the corrections \( \propto 1/m \) (instead of \( 1/m^2 \)), as illustrated in figure 6.

At least for even numbers of flavours a possible way out consists in adding a twisted mass term and setting \( m = 0 \). Then \( \gamma_5 \tau^1 (\bar{q} + i \mu_3 \gamma_5 \tau^3) \) is again hermitian. With this Dirac operator, the complementary field components at the boundaries satisfy simple Neumann conditions, and the spectrum is symmetric under a change of sign of the twisted mass term. A physically equivalent solution is obtained by staying with the standard mass term and rotating the boundary projectors instead. This will be discussed in more detail below. However, a caveat remains as only the simultaneous decoupling of an even number of quarks can be studied in this formalism. On the other hand, it may be sufficient to compare to perturbative decoupling in this slightly unphysical setting, in particular if a perturbative treatment turns out to be satisfactory.

### 8.3. SF boundary conditions and chiral rotations

Let us consider flavour doublets \( \psi' \) and \( \bar{\psi}' \) which satisfy homogeneous standard SF boundary conditions. Performing a chiral rotation,

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

one finds that the fields \( \psi \) and \( \bar{\psi} \) satisfy the chirally rotated boundary conditions,

\[ P_+ (\alpha) \psi(x) \big|_{x_0=0} = 0, \quad P_- (\alpha) \psi(x) \big|_{x_0=T} = 0, \]
\[ \bar{\psi}(x) \gamma_0 P_-(\alpha) \big|_{x_0=0} = 0, \quad \psi(x) \gamma_0 P_+ (\alpha) \big|_{x_0=T} = 0, \]

with the projectors,

\[ P_{\pm}(\alpha) = \frac{1}{2} [1 \pm \gamma_0 \exp(i \alpha \gamma_5 \tau^3)]. \]

Special cases are \( \alpha = 0 \) and \( \alpha = \pi/2 \) where one obtains,

\[ P_+ (0) = P_\pm, \quad P_\pm (\pi/2) \equiv Q_{\pm} = \frac{1}{2} (1 \pm i \gamma_0 \gamma_5 \tau^3). \]

We perform again a change of variables in the functional integral. Including mass terms as well, we label correlation functions by a subscript.
\[(m, \mu_q, P_+ (\alpha)), \text{ i.e. we include the projector defining the Dirichlet component of the quark field at } x_0 = 0. \text{ The generalisation of formula (22) then reads:}
\[
\langle O[\tilde{\psi}, \bar{\psi}](m, \mu_q, P_+) \rangle = \langle O[R(\alpha)\tilde{\psi}, \bar{\psi}R(\alpha)](\tilde{m}, \tilde{\mu}_q, P_+ (\alpha)) \rangle, \tag{75}
\]
with mass parameters \(\tilde{m}\) and \(\tilde{\mu}_q\) given by
\[
\tilde{m} = m \cos \alpha - \mu_q \sin \alpha, \quad \tilde{\mu}_q = m \sin \alpha + \mu_q \cos \alpha. \tag{76}
\]

The boundary quark fields are included in this transformation by replacing
\[
\tilde{\zeta}(\mathbf{x}) \leftrightarrow \bar{\psi}(0, \mathbf{x}) P_+, \quad \zeta(\mathbf{x}) \leftrightarrow P_- \psi(0, \mathbf{x}). \tag{77}
\]
This extends the equivalence between correlation functions of tmQCD and standard QCD to correlation functions derived from the Schrödinger functional. Simple examples are provided by purely gluonic observables \(O[U]\), such as the SF coupling constant. Eq. (75) then implies,
\[
\langle O[U](0, \mu_{R}, P_+) \rangle = \langle O[U](\mu_{R}, 0, Q_+) \rangle. \tag{78}
\]
In other words, either the mass term is twisted and one stays with standard SF boundary conditions, or the mass term is standard and the boundary conditions are fully twisted. In both cases one expects a quadratic dependence on the mass parameter and hence a relatively fast decoupling of heavy quarks.

### 8.4. SF schemes with Wilson quarks and \(O(a)\) improvement

From the discussion of \(O(a)\) improvement in section 6 one may conclude that \(\gamma_5 \tau^1\)-even observables computed with Wilson quarks in a finite volume and with periodic boundary conditions are automatically \(O(a)\) improved at zero quark mass. As SF schemes are usually defined at zero quark mass, it seems natural to ask how the SF boundary conditions interfere with this property. It is useful to think of \(O(a)\) effects to arise from different sources. First there are the \(O(a)\) boundary effects, which are cancelled by introducing the \(O(a)\) boundary counterterms to the action and the boundary quark and antiquark fields. Second there are \(O(a)\) effects from the bulk action which may be cancelled by the Sheikholeslami-Wohlert term, and third there are the \(O(a)\) effects associated with the composite operators in a given correlation function. It is interesting to note that \(O(a)\) cutoff effects from the bulk action are often quite large in SF correlation functions. This is illustrated in figure 7 which shows the relative cutoff effects in the perturbative one-loop coefficient of the step-scaling function of the
four-quark operator needed for $B_K$. The operator here is unimproved, and the boundary effects remain uncancelled in order to mimic the non-perturbative procedure of $5^3$. The most dramatic reduction of cutoff effects occurs when the Sheikholeslami-Wohlert term is included. Moreover, this has the side effect to reduce the ambiguity in the zero mass point, so that with the standard SF it makes sense to implement $O(a)$ improvement even if it is not complete.

![Figure 7](image-url)

Figure 7. Relative cutoff effects in the one-loop coefficient of the step-scaling function of the $B_K$ operator. Shown are two different regularizations ($c_{SW} = 0, 1$) with two definitions of the zero mass point.

### 8.5. The Schrödinger functional and $O(a)$ improvement

The reason why automatic $O(a)$ improvement fails is that the $\gamma_5 \tau^1$-transformation (54) changes the projectors of the quark boundary conditions,

$$P_{\pm} \gamma_5 \tau^1 = \gamma_5 \tau^1 P_{\mp}.$$ (79)
The boundary conditions, just like mass terms, define a direction in chiral flavour space. This means that the $\gamma_5 \tau^1$-transformation yields inequivalent correlation functions even in the chiral limit. For a $\gamma_5 \tau^1$-even operator $O$ one finds

$$\langle O \rangle_{(m, \mu_q, P^+)} \rightarrow \langle O \rangle_{(-m, \mu_q, P^-)}.$$  

(80)

It thus appears that the standard SF does not allow for the definition of $\gamma_5 \tau^1$-even correlation functions, and bulk $O(a)$ improvement is not automatic.

A possible solution is obtained by changing the projectors used to specify the Dirichlet components such that they commute with $\gamma_5 \tau^1$. Allowing for an additional flavour structure one may think of

$$Q_{\pm} = \frac{1}{2}(1 \pm i \gamma_0 \gamma_5 \tau^3).$$  

(81)

Interestingly, the projectors $Q_{\pm}$ also appear in the chiral rotation of the SF by $\alpha = \pi/2$. Besides automatic $O(a)$ improvement, the implementation of these boundary conditions may lead to some interesting checks of universality by comparing SF correlation functions in the standard framework and at maximal twist. Note that this direct comparison was not possible in 3,54, where a twisted mass term was introduced whilst keeping the standard SF boundary conditions.

8.6. The SF with chirally rotated boundary conditions

The implementation of some given boundary conditions is not straightforward on the lattice, and some care has to be taken to ensure that one really ends up with the desired continuum theory. A successful implementation of the maximally twisted boundary conditions involving the projectors $Q_{\pm}$ has been described in 55, and relies on an orbifold construction to ensure the correct continuum limit.

8.6.1. Symmetries and Counterterms

Apart from the absence of a dimensionful parameter, the symmetries of the SF with maximally twisted boundary conditions are identical to those of tmQCD. One may then list the possible boundary counterterms of dimension 3 allowed by the symmetries:

$$K_1 = \bar{\psi} i \gamma_5 \tau^3 \psi, \quad K_{\pm} = \bar{\psi} Q_{\pm} \psi.$$  

(82)

As time reflection combined with a flavour permutation is a symmetry of the SF, it is enough to discuss the counterterms at $x_0 = 0$. $K_1$ corresponds
to the logarithmically divergent boundary counterterm in the standard SF, which leads to a multiplicative renormalization of the quark boundary fields. The operator $K_+$ only involves Dirichlet components at $x_0 = 0$ and is therefore irrelevant for most correlation functions used in practice. The remaining operator $K_-$ only contains non-Dirichlet boundary components. If rotated back to the primed basis it becomes proportional to $\bar{\psi} i \gamma_5 \tau^3 P_- \psi'$, which violates flavour symmetry and parity just like a twisted mass term. As these are symmetries which are restored in the continuum limit one concludes that this counterterm must be scale-independent. Its coefficient can be fixed by requiring that a parity violating SF correlation function vanishes at finite $a$.

This analysis can be extended to dimension 4 operators which appear as $O(a)$ boundary counterterms. It turns out that the situation is comparable to the standard SF, i.e. there are a couple of counterterms which one needs to tune in order to eliminate the $O(a)$ boundary artefacts.

### 8.7. An example from perturbation theory

In perturbation theory, the values of all boundary counterterms are known, so that one may study both the equality of properly matched standard and twisted SF correlation functions, and confirm automatic bulk $O(a)$ improvement. A first example is given by the SF coupling, which can be related perturbatively to the MS-coupling,

$$\tilde{g}^2(L) = g_{\text{MS}}^2(\mu) + k_1(\mu L) g_{\text{MS}}^2(\mu) + O(g^6).$$

(83)

The fermionic contribution to the one-loop coefficient, $k_1 = k_{1,0} + N_f k_{1,1}$, has been computed in $^49$, yielding $k_{1,1} = -0.039863(2)/(4\pi)$. In practice, the perturbative data is obtained for a sequence of lattices, and one then expects the asymptotic large $L/a$ behaviour:

$$f(L/a) \sim r_0 + (a/L)[r_1 + s_1 \ln(a/L)] + O(a^2).$$

(84)

Here $r_0 = k_{1,1}$ is the continuum limit value, and the $O(a)$ effects lead to non-vanishing values of $r_1$ and $s_1$. In the standard Schrödinger functional set-up one expects that $r_1$ is eliminated by the boundary counterterm proportional to $\text{tr}(F_{0k} F_{0k})$, whereas $s_1$ is due to bulk $O(a)$ effects from the action, and thus proportional to $c_{sw}^{(0)} - 1$. On the other hand, with twisted SF boundary conditions one expects that $r_0$ remains the same, due to universality, $r_1$ is cancelled again by a boundary counterterm, and $s_1$ should vanish independently of the value of $c_{sw}^{(0)}$. This expectation is indeed confirmed numerically. A similar test can be performed with the tree level
quark propagator in a non-vanishing gauge background field, induced by choosing non-vanishing gauge field boundary values $C_k$ and $C'_k$. One then expects that, with the correct tree-level boundary counterterms, the bulk $O(a)$ lattice artefacts will again be either proportional to $c_{sw}^{(0)} - 1$ (standard SF) or absent (twisted SF). Again this expectation is confirmed. However, in contrast to the SF coupling this test can not be extended beyond the tree level, unless one fixes the gauge.

9. Conclusions

Lattice QCD with Wilson type quarks remains an attractive regularisation of lattice QCD. Some of its problems can be alleviated by introducing a chirally twisted quark mass term. While the theories remain equivalent in the continuum limit, the twisted mass term supplies an infrared bound on the spectrum of the Wilson-Dirac operator which renders the quenched and partially quenched approximations well-defined. Some of the notorious lattice renormalisation problems of standard Wilson quarks can be by-passed, and tmQCD at maximal twist is automatically $O(a)$ improved. These advantages are balanced by parity and flavour breaking and the fact that tmQCD comes naturally with an even number of quarks.

The Schrödinger functional has become an indispensable tool to tackle non-perturbative renormalisation problems in lattice QCD. However, the standard set-up leads to a slow decoupling of heavy quarks, and is in conflict with automatic $O(a)$ improvement of massless Wilson quarks. This motivates the application of a chiral twist to the SF boundary conditions. It is thus possible to extend equivalence between tmQCD and standard QCD to correlation functions derived from the Schrödinger functional. This allows for interesting tests of universality and the maximally twisted SF is compatible with automatic $O(a)$ improvement, as I have illustrated with simple perturbative examples.

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