Twisted mass QCD and lattice approaches to the $\Delta I = 1/2$ rule

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Abstract

Twisted mass lattice QCD (tmQCD), generalised to four Wilson quark flavours, can be used for the computation of some weak matrix elements related to $\Delta I = 1/2$ transitions. Besides eliminating unphysical zero modes, tmQCD may alleviate the four-quark operator renormalisation problems encountered in the calculation of CP-conserving $K \to \pi$ matrix elements with traditional Wilson fermion regularisation. With an active charm quark, the renormalisation of the $K \to \pi$ matrix elements requires at most the subtraction of a linearly divergent counterterm. Furthermore, in the (partially) quenched approximation the twist angles can be chosen so that only a finite counterterm needs to be subtracted.

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1 Introduction

In the phenomenology of non-leptonic kaon and hyperon decays, the observed enhancement of decays with isospin change $\Delta I = 1/2$ over those with $\Delta I = 3/2$ is referred to as the $\Delta I = 1/2$ rule. For example, $K^0$ decays into a pion pair of definite isospin $I$ can be parameterised through

$$A(K^0 \to (\pi\pi)_I) = A_I e^{i\delta_I},$$

(1.1)

where $\delta_I$ are the S-wave $\pi\pi$ phase shifts. The $\Delta I = 1/2$ rule manifests itself in the large value of the ratio

$$|A_0/A_2| \approx 22.$$  

(1.2)

Although the exact origin of this enhancement is unclear, it is believed that it must be related to long-distance, non-perturbative physics. The contribution coming from energy scales where perturbation theory can be reliably applied supplies only a small fraction of this ratio$^1$. The rest should be an effect characteristic of low-energy QCD scales. Analytic studies have provided only a partial understanding of this non-perturbative enhancement factor$^1$. It is fair to say that we are still far from a quantitative prediction based on QCD.

In principle, numerical simulations of lattice QCD are an ideal tool for the computation of the required hadronic matrix elements. Several lattice regularisations of the fermionic action has been used to this aim. We cite indicatively recent work performed with Wilson$^2$, staggered$^3$, and domain wall$^4$ fermions; for a more complete and fairly updated list of references, see ref.$^5$. In spite of the considerable effort invested in these simulations and several encouraging results, the ultimate goal is still far from being achieved, also because a number of conceptual and technical problems must be addressed beforehand.

First, the finite spatial volume, characteristic of lattice simulations, strongly affects the two-pion final state$^6$. In spite of this, it has been shown in$^7$ that physical $K \to \pi\pi$ matrix elements can nevertheless be obtained from Euclidean correlation functions, computed in a finite volume (see also$^8$ for a related approach). In particular a relation between the absolute values of the finite and infinite volume amplitudes is established. This, together with a separate measurement of the two-pion energies in finite volume, allows to fully reconstruct the desired decay amplitudes. However, the required spatial sizes $L$ still tend to be larger by a factor of 2-3 than the volumes typically used for the numerical determination of the hadronic spectrum.$^2$ Furthermore, unitarity is essential for the derivation of these results, so that the quenched approximation may

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$^1$The precise value depends on the renormalisation scheme used in the computation; e.g. in typical $\overline{\text{MS}}$ schemes it roughly amounts to a factor of two.

$^2$For a recent proposal, mitigating this requirement, see ref.$^9$.
not be applicable. Therefore, the practical feasibility of this programme hinges on possible theoretical developments, as well as further progress in simulation algorithms and computer hardware.

The difficulty of computing the physical amplitudes directly has led to less ambitious approaches, most of which aim at the determination of the coupling constants in the effective chiral Lagrangian \[10\]. This may be achieved by studying unphysical processes where no problem with final state interactions arises, such as \(K \rightarrow \pi\) transitions, or \(K \rightarrow \pi \pi\) decays with both pions at rest \[10]\,\[11]\,\[12\]. Once the effective coupling constants are known, the physical amplitudes can be inferred, up to higher order corrections in the chiral expansion. However, one might expect the next-to-leading order corrections to be large, especially if the matching to data from numerical simulations is performed at unphysically large meson masses. Assuming that the chiral expansion remains valid in this regime, it is thus desirable to include higher order terms in the chiral Lagrangian \[13]\,\[14\]. Unfortunately, since this introduces many more unknown parameters already at next-to-leading order, the whole approach becomes quite cumbersome if not impractical.

Whatever the chosen strategy, a difficult problem consists in the renormalisation of the four-quark operators which appear in the effective weak Hamiltonian. The details strongly depend on the symmetries of the lattice regularisation; regularisations which preserve chiral symmetry are clearly advantageous \[15]\,\[16]\,\[17\], and are increasingly used despite their high computational costs. If computationally cheaper quarks of the Wilson type are used instead, the operator renormalisation is complicated, mainly due to the presence of power divergences \[18]\,\[19\]. However, it should be noted that power divergences seem unavoidable, even with chirally symmetric regularisations, if the charm quark is not included as a dynamical degree of freedom in the low-energy approximation to the Standard Model.

In this paper we advocate the traditional approach of computing \(K \rightarrow \pi\) transitions, in a regime where lowest order chiral perturbation theory can be expected to work reliably. For chirally symmetric regularisations this requirement seems prohibitive, even in the quenched approximation, as the volume needs to be relatively large\(^3\). For Wilson-type fermions this problem is significantly less severe, but the renormalisation of the four-quark operators is very complicated. Even more importantly, in quenched simulations one is again forced to use relatively large meson masses, due to the presence of unphysical fermion zero modes. It is the purpose of the present paper to show that both the zero mode problem and the problem of operator renormalisation can be solved by using twisted mass QCD with four flavours of Wilson-type quarks. This could provide an affordable way of approaching the chiral regime by “brute force”, down to

\[^3\text{See, however, ref. [20] for an interesting alternative approach, where the effective theory is matched in a finite volume very close to the chiral limit.}\]
meson masses which are roughly twice the physical pion mass. In this regime the chiral expansion can be applied with confidence.

Since the arguments leading to our results are fairly complex, we have strived to present them in a detailed and fairly self-contained way. Moreover, in the conclusions we have summarised our findings in the form of recipes which can be applied in future numerical computations. Here we only wish to stress the underlying general principles which are at play behind the simplification of the renormalisation properties of the \( K \to \pi \) matrix elements in tmQCD. In this lattice regularisation, a twisted mass term is introduced in the Wilson fermion action. The ratio between the new (twisted) and the standard mass terms, expressed by “twist angles”, needs to be constrained in order to recover continuum QCD from the tmQCD regularisation. We are free to fix the twist angles to any value, but once the choice is made it is binding, in that it effectively labels a specific mode in which chirality is broken by the Wilson term. This in turn implies that a given operator is in general expressed in the twisted theory by a combination of all the components of its chiral multiplet. Since chiral symmetry is broken in the bare theory, each of these components has different renormalisation properties. Thus, judicious choices of the twist angles allow us to map the original operator into one of its chiral partners which has better renormalisation properties. This is exactly what happens in the case of the operators characteristic of \( K \to \pi \) transitions. We are able to map the original operator, which in the standard Wilson fermion regularisation has a quadratic divergence, into one which only has linear divergences. Since quadratic divergences are known to be prohibitively hard to subtract in non perturbative computations, while linear ones are well within our control, this is a significant gain. This softening of the divergence comes at a modest price: the twisted theory is characterised by soft symmetry breaking; in particular parity and isospin (in two directions of isospin space) are lost. Although these symmetries are recovered in the continuum limit, their breaking in the bare theory allows for more counterterms to come into play. In the case under consideration, the breaking of parity implies that one extra linearly divergent counterterm needs to be subtracted; i.e. an extra renormalisation condition must be imposed. This condition amounts to the restoration of parity as the continuum limit is taken. These considerations are valid in general. In more specific cases (choice of twist angles, improved action, quenched strange and charm quarks) we have shown that it is possible to avoid the linear subtraction altogether, by working with a pion source at large-time separations.

The layout of this paper is as follows. After a brief review of the effective weak Hamiltonian of the Standard Model, and the effective chiral theory at low energies (sect. 2), we recall the renormalisation properties of the relevant four-quark operators both in a chirally invariant regularisation and with standard Wilson quarks. In sect. 3 we introduce twisted mass QCD (tmQCD) with four quark flavours and establish the relations between its correlation functions and those of standard QCD. Renormalisation
and practical aspects of lattice regularised tmQCD are discussed in sect. 4. We are then prepared to describe strategies of how to extract $K \rightarrow \pi$ matrix elements (sect. 5) and we end with a short summary of our findings (sect. 6). This work has appeared in preliminary form in refs. [22].

2 The $\Delta I = 1/2$ rule and lattice QCD

In order to define the general framework we shortly review some aspects of the $\Delta S = 1$ effective weak Hamiltonian of the Standard Model, and its chiral effective theory in terms of kaons and pions.

2.1 Effective weak Hamiltonian

At scales well below $M_W$, but above the charm quark mass, weak, CP-conserving, $\Delta S = 1$ interactions can be described with an effective Hamiltonian of the form

$$H_{\text{eff}} = V_{ud} V_{us}^* \frac{G_F}{\sqrt{2}} \left[ C_+(\mu) O_R^+(\mu) + C_-^R(\mu) O_{R}^R(\mu) \right] + \text{h.c.}.$$  (2.1)

Here $O_R^\pm(\mu)$ are the four-fermion operators

$$O^\pm = \frac{1}{2} \left\{ (\bar{s}_L^\mu u^\mu)(\bar{u}_L^\mu d^\mu) \pm (\bar{s}_L^\mu d^\mu)(\bar{u}_L^\mu u^\mu) \right\} - [u \leftrightarrow c],$$  (2.2)

renormalised at a scale $\mu$ (the subscript R indicates renormalised operators), $C_\pm(\mu)$ are the corresponding Wilson coefficients, and $\gamma_{\mu}^L = \gamma_\mu(1 - \gamma_5)$. In principle, a further contribution to the weak Hamiltonian comes from integrating out the top quark. This has been neglected here, as it is suppressed by a factor $(V_{td} V_{ts}^*)/(V_{ud} V_{us}^*) = O(10^{-3})$.

The operators $O^\pm$ can be classified according to isospin symmetry as follows: $O^-$ is in the $I = 1/2$ representation, whereas $O^+$ is the sum of two contributions,

$$O^+ = O^+_{1/2} + O^+_{3/2},$$  (2.3)

corresponding to the representations with $I = 1/2$ and $I = 3/2$ respectively. These are given explicitly by

$$O^+_{1/2} = \frac{1}{6} \left[ (\bar{s}_L^\mu \mu u^\mu)(\bar{u}_L^\mu \mu d^\mu) + (\bar{s}_L^\mu \mu d^\mu)(\bar{u}_L^\mu \mu u^\mu) + 2(\bar{s}_L^\mu \mu d^\mu)(\bar{d}_L^\mu \mu d^\mu) \right]$$

$$- \frac{1}{2} \left[ (\bar{s}_L^\mu \mu c^\mu)(\bar{c}_L^\mu \mu d^\mu) + (\bar{s}_L^\mu \mu d^\mu)(\bar{c}_L^\mu \mu c^\mu) \right],$$  (2.4)

$$O^+_{3/2} = \frac{1}{3} \left[ (\bar{s}_L^\mu \mu u^\mu)(\bar{u}_L^\mu \mu d^\mu) + (\bar{s}_L^\mu \mu d^\mu)(\bar{u}_L^\mu \mu u^\mu) - (\bar{s}_L^\mu \mu d^\mu)(\bar{d}_L^\mu \mu d^\mu) \right].$$  (2.5)

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4We follow the standard convention and include effective quark bilinear operators as counterterms in the renormalised four-quark operators.
The $\Delta I = 1/2$ rule implies that the contribution of the $I = 1/2$ component of the effective Hamiltonian to $K \rightarrow \pi \pi$ matrix elements is much larger than that of its $I = 3/2$ part. This contradicts naive expectations and results in the $1/N_c$ expansion (cf. [23]).

Due to the chiral structure of the weak interactions, the operators or the effective Hamiltonian transform as singlets under the SU(3)$_R$ part of the chiral flavour group. Their classification according to the irreducible octet and 27-plet representations of SU(3)$_L$ can be found e.g. in ref. [20]. Here we note that we will be interested in regularisations with Wilson quarks and non-standard mass terms, which partially break the chiral flavour symmetries. The decomposition of the renormalised operators into irreducible chiral representations is then non-trivial and hence of limited use.

### 2.2 Effective chiral theory of kaons and pions

At low energies kaons and pions are the relevant degrees of freedom, and their interactions can be described by chiral perturbation theory (χPT) [24], in terms of the (Euclidean) action

$$S_{\text{eff}} = \int d^4x \frac{F^2}{4} \left\{ \text{Tr} \left( \partial_\mu U \partial_\mu U^\dagger \right) - \text{Tr} \left( U \chi^\dagger + \chi U^\dagger \right) \right\}.$$  \hspace{1cm} (2.6)

Here, $F$ is the the pseudoscalar meson decay constant, normalised so that $F_\pi = 92.4$ MeV is the experimental value determined from pion decay. The SU(3) matrix field $U(x)$ collects the pion, kaon and eta fields, parameterised as

$$U(x) = \exp(\sqrt{2}i\Phi(x)/F),$$  \hspace{1cm} (2.7)

with

$$\Phi = \begin{pmatrix} \pi^0/\sqrt{2} + \eta/\sqrt{6} & \pi^+ & K^+ \\ \pi^- & -\pi^0/\sqrt{2} + \eta/\sqrt{6} & K^0 \\ K^- & K^0 & -2\eta/\sqrt{6} \end{pmatrix}.$$  \hspace{1cm} (2.8)

A chiral flavour transformation $(g_L, g_R) \in SU(3)_L \times SU(3)_R$ transforms the $U$-field according to

$$U \rightarrow g_L U g_R^\dagger,$$  \hspace{1cm} (2.9)

and the action is invariant under this symmetry, provided the spurion field $\chi$ transforms in the same way as $U$. The symmetry is broken explicitly by setting

$$\chi = 2B\mathcal{M}, \quad \mathcal{M} = \text{diag}(m_u, m_d, m_s),$$  \hspace{1cm} (2.10)

where $B$ is a constant. Assuming isospin symmetry, $m_u = m_d = \hat{m}$, and expanding the $U$-field in powers of $\Phi$, one finds the lowest order relation between meson masses and quark masses,

$$m_\pi^2 = 2B\hat{m}, \quad m_K^2 = B(m_s + \hat{m}),$$  \hspace{1cm} (2.11)
which implies,
\[ \chi = \text{diag}(m_{\pi}^2, m_{\pi}^2, 2m_K^2 - m_{\pi}^2). \]  
(2.12)

The weak vertices for \( \Delta S = 1 \) processes which correspond to the effective 4-quark operators in the Standard Model can now be identified by their transformation behaviour under the chiral flavour symmetry. Following the conventions of [20] we have

\[ \mathcal{H}_w(x) = 2\sqrt{2}G_FV_{ud}V_{us}^\ast \left\{ \frac{5}{3}g_{27}\mathcal{O}_{27}(x) + 2g_8\mathcal{O}_{8}(x) + 2g'_8\mathcal{O}'_{8}(x) \right\} + \text{h.c.}. \]  
(2.13)

Using the notation
\[ L_\mu = \frac{F^2}{2}\partial_\mu U U^\dagger, \]  
(2.14)

the operators are explicitly given by

\[ \mathcal{O}_{27} = \frac{3}{5}(L_\mu)_{23}(L_\mu)_{11} + \frac{2}{5}(L_\mu)_{21}(L_\mu)_{13}, \]  
(2.15)

\[ \mathcal{O}_{8} = \frac{1}{2}\sum_{k=1}^{3}(L_\mu)_{2k}(L_\mu)_{k3}, \]  
(2.16)

\[ \mathcal{O}'_{8} = \frac{1}{4}F^4(U\chi U^\dagger + \chi U^\dagger)_{23}. \]  
(2.17)

Besides the parameters \( F \) and \( B \), first order \( \chi \)PT for electroweak processes of \( \Delta S = 1 \) contains the undetermined couplings \( g_{27}, g_8 \) and \( g'_8 \). Moreover, it can be shown that the so-called weak mass term proportional to \( g'_8 \) does not contribute to physical kaon decay amplitudes [10,25].

By matching experimental results for \( K \to \pi\pi \) decays to the rates obtained at lowest order chiral perturbation theory one may obtain a phenomenological estimate of \( g_8 \) and \( g_{27} \). Taking into account experimental information about the scattering phases between the pions in the final state, the authors of refs. [23,26] obtained the values
\[ |g_8| \approx 5.1, \quad |g_{27}| \approx 0.29. \]  
(2.18)

The clear hierarchy between the couplings reflects the \( \Delta I = 1/2 \) rule in the framework of leading order chiral perturbation theory.

2.3 \( K \to \pi \) amplitudes

An explanation of the \( \Delta I = 1/2 \) rule in this framework requires the determination of the couplings \( g_8 \) and \( g_{27} \) directly from QCD. Instead of a direct determination of the physical \( K \to \pi\pi \) transitions, it has become customary to study the unphysical
$K \to \pi$ amplitudes \cite{10}. Using standard conventions (see e.g \cite{27}) the matrix element for $K^+ \to \pi^+$ transitions in the effective theory is

$$\langle \pi^+, q | H_w(0) | K^+, p \rangle = \sqrt{2} G_F V_{ud} V_{us}^* F^2 \left\{ \left( \frac{2}{3} g_{27} + g_8 \right) p \cdot q + 2m_K^2 g_8' \right\}, \quad (2.19)$$

where

$$p \cdot q = E_K(p) E_\pi(q) - p \cdot q, \quad E_X(p) = \sqrt{m_X^2 + p^2}. \quad (2.20)$$

In order to determine the combination $\frac{2}{3} g_{27} + g_8$ we note that this term is proportional to the product of spatial momenta $p \cdot q$, while the unwanted $g_8'$ term is part of the $m_K^2$ contribution. One could thus isolate the former term by e.g. evaluating the $K^+ \to \pi^+$ matrix element in lattice QCD for two different pion energies (i.e. two different sets of spatial momenta). A technical disadvantage of this approach (as opposed to the one adopted with domain wall fermions in \cite{11}) is that it requires computation of lattice correlation functions with non-zero spatial momenta, which are noisy.

In order to obtain both $g_{27}$ and $g_8$ independently one then needs a second matrix element. If isospin symmetry is unbroken on the lattice, one may use the decomposition \cite{2.3} and the corresponding one in the effective theory, where the octet operator only mediates transitions with $\Delta I = 1/2$, whereas the 27-plet operator contains both, $\Delta I = 1/2$ and $3/2$. Decomposing this operator

$$O_{27} = O_{27}^{1/2} + O_{27}^{3/2}, \quad (2.21)$$

with

$$O_{27}^{1/2} = \frac{1}{15} \left[ (L_\mu)_{21} (L_\mu)_{13} + (L_\mu)_{23} \{4(L_\mu)_{11} + 5(L_\mu)_{22}\} \right], \quad (2.22)$$

$$O_{27}^{3/2} = \frac{1}{3} \left[ (L_\mu)_{21} (L_\mu)_{13} + (L_\mu)_{23} \{(L_\mu)_{11} - (L_\mu)_{22}\} \right], \quad (2.23)$$

it is easy to check that the $K^+ \to \pi^+$ matrix elements of these operators yield two independent combinations of $g_8$ and $g_{27}$. If isospin is not a lattice symmetry the isospin decomposition of the lattice operators poses a difficult renormalisation problem by itself. Rather than addressing this problem, one may instead look at the $K^0 \to \pi^0$ matrix element,

$$\langle \pi^0, q | H_w(0) | K^0, p \rangle = G_F V_{ud} V_{us}^* F^2 \left\{ (g_{27} - g_8) p \cdot q - 2m_K^2 g_8' \right\}, \quad (2.24)$$

which yields the combination $g_{27} - g_8$. However, we anticipate that this matrix element may be difficult to evaluate in twisted mass lattice QCD (cf. sect. 5.6).

Finally we recall the fact that $g_{27}$ can be related, via chiral symmetry, to $B_K$ in the chiral limit. Using an independent determination of $B_K$ as input, one may subsequently obtain $g_8$ by studying the $K^+ \to \pi^+$ matrix element of eq. (2.19).
2.4 Renormalisation of the four-quark operators on the lattice

In practice the renormalisation of the four-quark operators has been one of the major stumbling blocks for lattice regularisations which do not preserve chiral symmetry, such as lattice QCD with Wilson type quarks [28]. Decomposing the operators \( O^\pm \) into parity-even and parity-odd parts,

\[
O^\pm = O^\pm_{VV+AA} - O^\pm_{VA+AV},
\]

we see that parity ensures that \( K \to \pi\pi \) matrix elements receive contributions only from \( O^\pm_{VA+AV} \), while \( K \to \pi \) matrix elements arise only from \( O^\pm_{VV+AA} \).

To illustrate the importance of chiral symmetry we briefly recall the counterterm structure in the case of an ideal regularisation with cutoff \( 1/a \), in the sense that the continuum symmetries are preserved (see e.g. [29]). In this case one finds that the operators renormalise as follows:

\[
(O_R)^{\pm}_{VA+AV} = Z^{\pm}_{VA+AV}[O^\pm_{VA+AV} + c^\pm (m^2_c - m^2_u) (m_s - m_d) \bar{s}\gamma_5 d], \tag{2.26}
\]

\[
(O_R)^{\pm}_{VV+AA} = Z^{\pm}_{VV+AA}[O^\pm_{VV+AA} + c^\pm (m^2_c - m^2_u) (m_s + m_d) \bar{s}d]. \tag{2.27}
\]

Here, the multiplicative renormalisation constants \( Z^{\pm} \) and the additive renormalisation constants \( c^\pm \) are the same for both operators. Counterterms which vanish by the equations of motion have been omitted. This is justified as long as only on-shell correlation functions are considered. Note that lattice regularisations with Ginsparg-Wilson fermions provide explicit examples for the ideal regularisation, if one disregards the breaking of the continuous space-time symmetries. Therefore, with Ginsparg-Wilson fermions, the renormalisation pattern of the operators can indeed be cast in the form [2.26, 2.27] [10]. Furthermore, one expects that the operators are on-shell \( O(a) \) improved, i.e. leading cutoff effects in their matrix elements are of \( O(a^2) \).

In contrast, for Wilson-type quarks one finds the counterterm structure (see e.g. [19] [28] [12])

\[
(O_R)^{\pm}_{VA+AV} = Z^{\pm}_{VA+AV}[O^\pm_{VA+AV} + c^\pm_P \bar{s}\gamma_5 d], \tag{2.28}
\]

\[
(O_R)^{\pm}_{VV+AA} = Z^{\pm}_{VV+AA}[\sum_{k=1}^{5} Z^\pm_k O^\pm_k + c^\pm_S \bar{s}d + d^\pm S\bar{s}\sigma_{\mu\nu} F_{\mu\nu} d]. \tag{2.29}
\]

Here \( k \in \{VV + AA, VV - AA, SS, PP, TT\} \) labels the parity even Dirac structures of the four-quark operators in standard notation [29], and \( F_{\mu\nu} \) denotes some lattice version of the gluon field strength tensor. Once more, counterterms which vanish by the equations of motion have been neglected.
A first observation is that the parity even and odd operators are renormalised differently. Compared to the chirally symmetric regularisation one also finds that some of the additive renormalisation constants are divergent as $a \to 0$:

\[
\begin{align*}
    c_P^\pm & \sim \frac{1}{a} (m_c - m_u) (m_s - m_d), \\
    c_S^\pm & \sim \frac{1}{a^2} (m_c - m_u), \\
    d_\sigma^\pm & \sim (m_c - m_u). 
\end{align*}
\]

This is due to the loss of a factor $(m_c + m_u)$ and, for the parity even operator, of a further factor $(m_s + m_d)$. Instead of a finite counterterm one now has linear and quadratic divergences for the parity odd and even operators respectively. In the latter case there is also a subleading finite counterterm. An additional complication arises in the parity even operator due to the mixing with four other operators of dimension 6. Finally, we note that the renormalised operators are not $O(a)$ improved. These complicated renormalisation properties of the parity even operator have prevented the computation of $K \to \pi$ transitions with Wilson fermions \cite{28}. On the other hand, the situation for the parity odd operator is not much worse than the case of a chirally symmetric regularisation: only a single additive counterterm needs to be subtracted (besides the multiplicative renormalisation). This motivates us to investigate whether twisted mass QCD may alleviate the lattice renormalisation problem, in a similar way as discussed for $F_\pi$ and the matrix element for $K^0 - \bar{K}^0$ mixing in refs. \cite{30,31,32}.

3 Twisted mass QCD with four quark flavours

Twisted mass QCD has been designed to eliminate exceptional configurations in (partially) quenched lattice simulations with light Wilson quarks \cite{30}. In its original formulation, it describes a mass-degenerate isospin doublet $\psi$ of Wilson quarks for which, besides the standard mass term, a so-called twisted mass term $i\mu_q \bar{\psi} \gamma_5 \tau^3 \psi$ is introduced. The properties of tmQCD have been studied in detail in \cite{31}, where, in particular, its equivalence to standard two-flavour QCD has been established. We discuss here the extension of this framework to four quark flavours.

3.1 Classical action

We start by considering tmQCD in the continuum with the fermionic action

\[
S_F = \int d^4x \bar{\psi}(x) \left( D_\mu \gamma_\mu + m + i\gamma_5 \mu \right) \psi(x),
\]
where, $\psi^T = (u, d, s, c)$. The standard and twisted mass matrices have the form, respectively:

$$
\mathbf{m} = \text{diag} \left( M_u \cos \alpha, M_d \cos \alpha, M_s \cos \beta, M_c \cos \beta \right)
\equiv \text{diag}(m_u, m_d, m_s, m_c),
$$

$$
\mathbf{\mu} = \text{diag} \left( M_u \sin \alpha, -M_d \sin \alpha, M_s \sin \beta, -M_c \sin \beta \right)
\equiv \text{diag}(\mu_u, \mu_d, \mu_s, \mu_c).
$$

(3.2) (3.3)

Hence the theory has six independent parameters, namely the four radial quark masses $M_i$ ($i = u, d, s, c$), with $M_i^2 = m_i^2 + \mu_i^2$, and the two twist angles $\alpha, \beta$. In other words, the four standard mass parameters $m_i$ and the four twisted mass parameters $\mu_i$ are constrained by

$$
\tan \alpha = \frac{\mu_u}{m_u} = -\frac{\mu_d}{m_d}, \quad \tan \beta = \frac{\mu_s}{m_s} = -\frac{\mu_c}{m_c}.
$$

(3.4)

This framework is a natural extension of two-flavour tmQCD, with the property that the quark mass terms remain flavour diagonal. At vanishing twist angles $\alpha$ and $\beta$ one recovers the standard QCD action of four quark flavours, while for $\beta = 0$ and $M_u = M_d$ the two-flavour version of tmQCD of ref. [31] is reproduced, with two additional untwisted quark flavours $s$ and $c$.

The action (3.1) is form invariant under the axial field transformations

$$
\psi \rightarrow \psi' = R(\tilde{\alpha}, \tilde{\beta})\psi, \quad \bar{\psi} \rightarrow \bar{\psi}' = \bar{\psi}R(\tilde{\alpha}, \tilde{\beta}),
$$

(3.5)

with

$$
R(\tilde{\alpha}, \tilde{\beta}) = \exp \left\{ \frac{i}{2}\gamma_5 \left( \tilde{\alpha} \tau_3^l + \tilde{\beta} \tau_3^h \right) \right\},
$$

(3.6)

$$
\tau_3^l = \text{diag}(1, -1, 0, 0), \quad \tau_3^h = \text{diag}(0, 0, 1, -1).
$$

(3.7) (3.8)

The new mass term is given by

$$
\mathbf{m}' + i\gamma_5 \mathbf{\mu}' = R(2\tilde{\alpha}, 2\tilde{\beta}) \left[ \mathbf{m} + i\gamma_5 \mathbf{\mu} \right],
$$

(3.9)

and can again be parameterised as in eqs. (3.2,3.3). The corresponding twist angles $(\alpha', \beta') = (\alpha - \tilde{\alpha}, \beta - \tilde{\beta})$ are related to the mass parameters $\mathbf{m}', \mathbf{\mu}'$ as in eq. (3.4).

The radial masses $M_i$ remain invariant. With the choice $\tilde{\alpha} = \alpha, \tilde{\beta} = \beta$ one obtains $\mathbf{\mu}' = 0$ and $\mathbf{m}' = \text{diag}(M_u, M_d, M_s, M_c)$, i.e. four-flavour QCD with a standard mass term. This demonstrates the equivalence of tmQCD and standard QCD at the level of the classical action. It also implies that both theories share all the symmetries. For example, a parity transformation, $x \rightarrow \tilde{x} \equiv (x_0, -\mathbf{x})$, is realised in tmQCD by the field transformations

$$
\psi(x) \rightarrow \gamma_0 R(2\alpha, 2\beta) \psi(\tilde{x}), \quad \bar{\psi}(x) \rightarrow \bar{\psi}(\tilde{x})R(2\alpha, 2\beta) \gamma_0,
$$

(3.10)

with angles $\alpha, \beta$ given by eq. (3.4).
3.2 Relations between composite fields

In general, the axial transformation\(^{33}\) induces a mapping between composite fields. For quark bilinear operators, it can be written in a compact form:

\[\bar{\psi}_i \Gamma_j \psi_j = \cos(\phi_{ij}^\Gamma) \bar{\psi}_i' \Gamma_j \psi_j' + i \eta_{\Gamma} \sin(\phi_{ij}^\Gamma) \bar{\psi}_i' \Gamma_j \gamma_5 \psi_j'.\] (3.11)

Here we have assumed that the spin matrices \(\Gamma\) either commute or anticommute with \(\gamma_5\). The phases are then defined by

\[\phi_{ij}^\Gamma = \omega_i - \eta_{\Gamma} \omega_j, \quad \eta_{\Gamma} = \begin{cases} +1, & \text{if } \{\gamma_5, \Gamma\} = 0, \\ -1, & \text{if } [\gamma_5, \Gamma] = 0, \end{cases}\] (3.12)

and

\[\omega_u = -\omega_d = \frac{\tilde{\alpha}}{2}, \quad \omega_s = -\omega_c = \frac{\tilde{\beta}}{2}.\] (3.13)

These relations establish a “dictionary” between composite fields in theories with different parameterisations of the quark mass terms. As shown in ref.\(^{31}\) the very same relations hold between properly renormalised fields in the quantum theories, provided the renormalisation scheme respects the chiral and flavour symmetries of the massless continuum theory.

For illustration and later use we quote a few specific examples. With the notation for quark bilinear fields

\[S_{ij} = \bar{\psi}_i \psi_j, \quad P_{ij} = \bar{\psi}_i \gamma_5 \psi_j, \quad A_{\mu,ij} = \bar{\psi}_i \gamma_\mu \gamma_5 \psi_j, \quad V_{\mu,ij} = \bar{\psi}_i \gamma_\mu \psi_j,\] (3.14)

we find, for instance

\[S_{us} = \cos\left(\frac{\tilde{\alpha} + \tilde{\beta}}{2}\right) S_{us}' - i \sin\left(\frac{\tilde{\alpha} + \tilde{\beta}}{2}\right) P_{us}',\] (3.15)

\[P_{us} = \cos\left(\frac{\tilde{\alpha} + \tilde{\beta}}{2}\right) P_{us}' - i \sin\left(\frac{\tilde{\alpha} + \tilde{\beta}}{2}\right) S_{us}',\] (3.16)

\[A_{\mu,us} = \cos\left(\frac{\tilde{\alpha} - \tilde{\beta}}{2}\right) A_{\mu,us}' + i \sin\left(\frac{\tilde{\alpha} - \tilde{\beta}}{2}\right) V_{\mu,us}',\] (3.17)

\[V_{\mu,us} = \cos\left(\frac{\tilde{\alpha} - \tilde{\beta}}{2}\right) V_{\mu,us}' + i \sin\left(\frac{\tilde{\alpha} - \tilde{\beta}}{2}\right) A_{\mu,us}'.\] (3.18)

We observe that the axial transformation amounts to a rotation by the angle \((\tilde{\alpha} + \tilde{\beta})/2\) in the coordinates \((P_{us}, -i S_{us})\) and by the angle \((\tilde{\alpha} - \tilde{\beta})/2\) in the coordinates \((A_{us}, i V_{us})\). With a sign flip \(\tilde{\alpha} \rightarrow -\tilde{\alpha}\) the same equations hold if the up quark is replaced by a down quark. As for operators with up and down quarks only, we find

\[P_{du} = P_{du}', \quad A_\mu^3 = A_\mu'^3,\] (3.19)

where we have used the isospin notation

\[A_\mu^3 = \frac{1}{2} (A_{\mu,uu} - A_{\mu,dd}).\] (3.20)
3.3 Partial current conservation

With non-degenerate quark masses all chiral and flavour symmetries are broken explicitly. This is expressed by the non-vanishing r.h.s. of the PCAC and PCVC relations. For the flavour non-diagonal operators with $i \neq j$, they read,

$$
\partial_\mu A_{\mu,ij} = (m_i + m_j)P_{ij} + i(\mu_i + \mu_j)S_{ij},
\quad (3.21)
$$

$$
\partial_\mu V_{\mu,ij} = (m_i - m_j)S_{ij} + i(\mu_i - \mu_j)P_{ij}.
\quad (3.22)
$$

These relations take their usual form when expressed in terms of the axially transformed fields. Indeed, setting $\tilde{\alpha} = \alpha$ and $\tilde{\beta} = \beta$, the PCAC and PCVC relations become

$$
\partial_\mu A'_{\mu,ij} = (M_i + M_j)P'_{ij}, \quad \partial_\mu V'_{\mu,ij} = (M_i - M_j)S'_{ij}.
\quad (3.23)
$$

3.4 Mapping of four-quark operators

Using eq. (3.11) we obtain the relations for the four-quark operators of interest:

$$
O_{VV+AA}^\pm = \cos \left( \frac{\tilde{\alpha} + \tilde{\beta}}{2} \right) O_{VV+AA}^{\prime \pm} + i \sin \left( \frac{\tilde{\alpha} + \tilde{\beta}}{2} \right) O_{VA+AV}^{\prime \pm},
\quad (3.24)
$$

$$
O_{VA+AV}^\pm = \cos \left( \frac{\tilde{\alpha} + \tilde{\beta}}{2} \right) O_{VA+AV}^{\prime \pm} + i \sin \left( \frac{\tilde{\alpha} + \tilde{\beta}}{2} \right) O_{VV+AA}^{\prime \pm}.
\quad (3.25)
$$

The transformation is a rotation by the angle $(\tilde{\alpha} + \tilde{\beta})/2$ in the plane spanned by $(O_{VV+AA}^\pm, iO_{VA+AV}^\pm)$ and can be easily inverted by reversing the sign of the twist angles. Setting again $\tilde{\alpha} = \alpha$ and $\tilde{\beta} = \beta$ it is worth noting two special cases:

(i) $\alpha = \beta = \pi/2$: with this choice the operators are directly interchanged, as eqs. (3.24,3.25) become

$$
O_{VV+AA}^\pm = iO_{VA+AV}^{\prime \pm}, \quad O_{VA+AV}^\pm = iO_{VV+AA}^{\prime \pm}.
\quad (3.26)
$$

In terms of the quark masses these twist angles correspond to vanishing standard mass parameters,

$$
m_u = m_d = m_s = m_c = 0,
\quad (3.27)
$$

and positive twisted mass parameters for up and strange quarks.

(ii) $\alpha = -\beta = \pi/2$: in this case one finds

$$
O_{VV+AA}^\pm = O_{VV+AA}^{\prime \pm}, \quad O_{VA+AV}^\pm = O_{VA+AV}^{\prime \pm}.
\quad (3.28)
$$

In terms of quark masses the only difference with respect to the previous case is a change of sign for the twisted mass parameters of the strange and charm quarks.

We will refer to both these cases as “fully twisted”, since the physical quark masses $M_i$ are then determined by the twisted mass parameters alone. In the fully twisted cases the operator $O_{VA+AV}^\pm$ can play the rôle of either the parity even or the parity odd operator, depending on the sign of $\beta$. 

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3.5 Relations between correlation functions

Consider, in the formal continuum theory, Euclidean correlation functions of the form
\[ \langle O[\psi, \bar{\psi}] \rangle_{(\alpha, \beta)} = Z^{-1} \int_{\text{fields}} O[\psi, \bar{\psi}] e^{-S}, \]  
(3.29)

where \( O[\psi, \bar{\psi}] \) denotes some multilocal gauge invariant field. The fermionic part of the action is given in (3.1). Performing the field transformation eq. (3.5) and changing integration variables in the functional integral one derives the identity
\[ \langle O \left[ R(\tilde{\alpha}, \tilde{\beta}) \psi, \bar{\psi} R(\tilde{\alpha}, \tilde{\beta}) \right] \rangle_{(\alpha, \beta)} = \langle O \left[ \psi, \bar{\psi} \right] \rangle_{(\alpha-\tilde{\alpha}, \beta-\tilde{\beta})}, \]  
(3.30)

where the integration variables are \( \psi \) and \( \bar{\psi} \) on both sides of the equation, and the Jacobian is unity, due to
\[ \det \left( R(\tilde{\alpha}, \tilde{\beta}) \right) = 1. \]  
(3.31)

Setting \( \tilde{\alpha} = \alpha \) and \( \tilde{\beta} = \beta \) we thus obtain identities between standard QCD and twisted mass QCD correlation functions, which we can use in two alternative versions:
\[ \langle O \left[ \psi, \bar{\psi} \right] \rangle_{(\alpha, \beta)} = \langle O \left[ R(-\alpha, -\beta) \psi, \bar{\psi} R(-\alpha, -\beta) \right] \rangle_{(0, 0)}, \]  
(3.32)
\[ \langle O \left[ \psi, \bar{\psi} \right] \rangle_{(0, 0)} = \langle O \left[ R(\alpha, \beta) \psi, \bar{\psi} R(\alpha, \beta) \right] \rangle_{(\alpha, \beta)}. \]  
(3.33)

Hence, a given correlation function in tmQCD with twist angles \( (\alpha, \beta) \) is interpreted as the linear combination on the r.h.s. of eq. (3.32). If instead we are given a standard QCD correlation function, then eq. (3.33) tells us how it is represented in tmQCD at twist angles \( (\alpha, \beta) \). The dictionary just established for composite fields can be used for the integrands in eq. (3.32), provided \( \psi' \) and \( \bar{\psi}' \) are identified with the integration variables on the r.h.s.. As shown in ref. [31], the relations derived for the formal continuum theory are realised between the renormalised quantum field theories, provided the renormalisation procedure is set up with some care.

4 Lattice regularised tmQCD

To regularise tmQCD on the lattice, we assume that the gauge fields are represented by some standard lattice action (e.g. Wilson’s plaquette action), whereas quarks are described by the lattice action
\[ S_l = a^4 \sum_x \bar{\psi}(x) \left( D_W + m + i\gamma_5 \mu \right) \psi(x), \]  
(4.1)

with \( D_W \) being the standard, possibly \( O(a) \) improved Wilson-Dirac operator (for unexplained notation see [33]). In order to ensure the equivalence between tmQCD and
standard QCD, the bare mass parameters, \( m_i \) and \( \mu_i \) \((i = u, d, s, c)\), will be subject to constraints. However, these are now only implicitly defined by eqs. (3.4), as they will be imposed on the properly renormalised mass parameters. Before discussing renormalisation of lattice tmQCD we consider the possible choices for the bare mass parameters leading to feasible numerical simulations.

### 4.1 Quark determinant and practical choices of parameters

Whether a given lattice action is suitable for numerical simulations obviously depends on the available algorithms. The answer may therefore change with time. At present, the starting point for most algorithms is the functional integral after integration over the quark fields. The resulting determinant is then part of the effective gauge field measure and is generally required to be real and positive. In the case of lattice tmQCD with four quark flavours as introduced here, each flavour contributes a factor to the determinant. Assuming the light doublet to be mass degenerate,

\[
m_u = m_d = m_l, \quad \mu_u = -\mu_d = \mu_l,
\]

the determinants of the two light flavours can be combined to yield

\[
\det \left( D_W + m_l + i\mu_l \gamma_5 \tau^3 \right) = \det \left[ (D_W + m_l) \dagger (D_W + m_l) + \mu_l^2 \right],
\]

where the determinant on the r.h.s. is taken in a single flavour space. Hence the determinant of the light doublet is positive at non-zero \( \mu_l \), irrespective of the background gauge field. Integrating over strange and charm quarks one obtains

\[
\det \left[ (D_W + m_s) \dagger (D_W + m_c) - \mu_s \mu_c \right.
\]

\[
+ i \mu_c \gamma_5 \{ D_W + m_s \} + i \mu_s \gamma_5 \{ D_W + m_c \} \left],
\]

which, in general, is not a real quantity. Discarding the unphysical situation of mass-degenerate strange and charm quarks, the only way to ensure the reality of the determinant is to employ untwisted strange and charm quarks, \( \mu_s = \mu_c = 0 \), as the fermion determinants for individual Wilson quark flavours are real. However, positivity of the determinant is then not guaranteed, unless the quark masses are large enough. Detailed statements depend on the lattice gauge action and the chosen simulation parameters, but for practical purposes the strange quark mass might be heavy enough (see, e.g. [34]).

In view of this situation we distinguish the following practical options for lattice tmQCD simulations:

- Quenched simulations or partially quenched simulations with \( N_f = 2 \) dynamical light and mass degenerate quarks. Strange and charm quarks remain quenched
and do not contribute to the determinant, which is therefore guaranteed to be real and positive (for $\mu_l \neq 0$). Hence, one has almost complete freedom in the choice of the mass parameters and therefore of $\alpha$ and $\beta$. In the quenched approximation one would just require a non-zero twist angle $\alpha$ in order to ensure the absence of unphysical zero modes.

- $N_f = 3, 4$ dynamical quark flavours with two mass degenerate light quarks, and untwisted strange and charm quarks. This implies the choice for the second twist angle $\beta = 0$, while $\alpha$ remains unrestricted.

Note that these considerations pertain to our specific choice of flavour diagonal mass terms. If one allows for flavour non-diagonal mass terms one may indeed be able to obtain positive and real fermion determinants for any combination of non-zero quark masses, including non-degenerate light quarks [35]. However, this renders the relation between standard QCD and tmQCD correlation functions more complicated, and the flavour structure has to be dealt with explicitly in the numerical computation of quark propagators.

### 4.2 Renormalisation of lattice tmQCD

Renormalisability is based on general properties of Quantum Field Theory, such as locality and unitarity, which may not hold in the (partially) quenched approximation of QCD. In this paper we do not try to solve this general problem. Instead we take the naive point of view that the (partially) quenched theory is well-defined and can be obtained by suppressing the fermion determinant with respect to some or all flavours. This is assumed to incur no drastic change to the theory’s renormalisability. While we discuss the counterterm structure for the full theory with $N_f = 4$ dynamical quarks, we occasionally indicate modifications which should be expected in the (partially) quenched case.

#### 4.2.1 Symmetries of the lattice action

When the mass terms are taken to vanish, the tmQCD lattice action reduces to the usual (possibly $O(a)$ improved) Wilson action for $N_f = 4$ quarks. Hence, the massless tmQCD lattice action ($m = \mu = 0$) is invariant under $U(4)$ flavour rotations,

$$\psi \rightarrow V \psi, \quad \bar{\psi} \rightarrow \bar{\psi} V^\dagger,$$

as well as under discrete transformations, such as parity ($x \rightarrow \tilde{x} = (x_0, -x)$),

$$\psi(x) \rightarrow \gamma_0 \psi(\tilde{x}), \quad \bar{\psi} \rightarrow \bar{\psi}(\tilde{x}) \gamma_0,$$

(4.6)
and charge conjugation

$$\psi(x) \rightarrow C^{-1} \bar{\psi}(x)^T, \quad \bar{\psi} \rightarrow -\psi(x)^T C$$

(4.7)

(the charge conjugation matrix satisfies $\gamma^{\mu*} = -C \gamma^{\mu} C^{-1}$).

Once the mass and twisted mass terms are added, some of these symmetries are lost. The introduction of the $m$ term implies loss of the $U(4)$ flavour symmetry, unless $m \propto 1$. Upon introducing the $\mu$ term this symmetry is also lost. A reduced symmetry survives however, if $\mu \propto \text{diag}(1, -1, 1, -1)$. This consists of isospin rotations of the $SU(2)$ subgroups, along the generators $\tau_3^l$ and $\tau_3^h$ defined in eqs. (3.7) and (3.8). Charge conjugation is unaffected by the mass terms, while parity is clearly broken by the twisted mass term.\(^5\)

Upon adding the two mass terms, one may determine the counterterm structure by treating $m$ and $\mu$ as spurion fields which transform under these symmetries so that the massive theory remains formally invariant. In particular, under a $U(4)$ flavour transformation (4.5) one assumes that

$$m \rightarrow V m V^\dagger, \quad \mu \rightarrow V \mu V^\dagger,$$

(4.8)

while invariance under the parity transformation (4.6) is obtained by assuming

$$m \rightarrow m, \quad \mu \rightarrow -\mu.$$  

(4.9)

However, we stress again that in tmQCD with Wilson quarks and nonvanishing twisted masses physical parity, as defined in eq. (3.10), is broken at $O(a)$, and is recovered only in the continuum limit. Analogous considerations hold in the case of the $U(4)$ vector flavour symmetry.

It is sometimes useful to restrict attention to a subset of the general flavour transformations (4.5), such as flavour exchanges

$$\psi_i \leftrightarrow \psi_j, \quad \bar{\psi}_i \leftrightarrow \bar{\psi}_j,$$

(4.10)

for which the spurion transformations (4.8) reduce to an exchange of the corresponding mass parameters,

$$m_i \leftrightarrow m_j, \quad \mu_i \leftrightarrow \mu_j.$$  

(4.11)

\(^5\)We have not indicated the parity and charge conjugation transformations of the gauge field, as they are never used in this work.

\(^6\)The reader should not be misled by the fact that the redefined parity transformation is a symmetry of the classical action. Although the $\mu$ term is invariant under this symmetry, the Wilson term is not.
4.2.2 Renormalised parameters

The physical interpretation of tmQCD hinges on the knowledge of the twist angles in the renormalised theory. As these are determined by ratios of the renormalised standard and twisted mass parameters we first discuss renormalisation of the bare parameters in the action.

The counterterms to the action of dimension \( \leq 4 \) are,

\[
\text{tr} \{ F_{\mu\nu} F^{\mu\nu} \}, \quad \bar{\psi} \psi, \quad \text{tr}(m) \bar{\psi} \psi, \quad i \text{tr}(\mu) \bar{\psi} \gamma_5 \psi, \quad i \bar{\psi} \mu \gamma_5 \psi,
\]

where \( F_{\mu\nu} \) denotes the gluon field strength tensor. The first counterterm implies a multiplicative renormalisation of the bare gauge coupling. As for the quark mass renormalisation the situation is complicated by the trace terms, which would be absent in a chirally symmetric regularisation. For standard Wilson fermions the situation has been discussed in refs. [36,37], which can be summarised and extended as follows: first one decomposes the mass matrices in non-singlet and singlet pieces,

\[
m = \sum_{a=1}^{15} m^a \lambda^a + m^0 \mathbb{1}_4, \quad \mu = \sum_{a=1}^{15} \mu^a \lambda^a + \mu^0 \mathbb{1}_4,
\]

where \( \lambda^a \), \( a = 1, \ldots, 15 \) are the generators of SU(4). This decomposition applies to general Hermitean \( 4 \times 4 \) matrices, but with our choice of flavour diagonal mass matrices only 3 of the non-singlet coefficients are non-zero. These correspond to the 3 diagonal and traceless generators of SU(4) and are therefore linear combinations of (twisted) mass differences. The singlet coefficients are given by

\[
m^0 = \frac{1}{4} \text{tr}(m), \quad \mu^0 = \frac{1}{4} \text{tr}(\mu),
\]

The non-singlet terms are renormalised by the inverse renormalisation constant of the non-singlet scalar and pseudoscalar densities, \( S_{ij} \) and \( P_{ij} \) \((i \neq j)\) respectively,

\[
m_R^a = Z_S^{-1} m^a, \quad \mu_R^a = Z_P^{-1} \mu^a.
\]

The renormalised singlet masses \( m^0 \) and \( \mu^0 \) are then given by

\[
m_R^0 = Z_S^{-1} (m^0 - m_c), \quad \mu_R^0 = Z_P^{-1} \mu^0,
\]

where \( Z_{S^0, P^0} \) are the multiplicative renormalisation constants of the singlet densities \( S^0 = \sum_{i=1}^{4} S_{ii} \) and \( P^0 = \sum_{i=1}^{4} P_{ii} \) respectively, and \( m_c \) denotes the “critical mass”.

From this renormalisation pattern we obtain for quark mass parameters of individual flavours

\[
m_{R,i} = Z_S^{-1} \left[ m_i - m_c + (r_m - 1) (m^0 - m_c) \right], \quad \mu_{R,i} = Z_P^{-1} \left[ \mu_i + (r_\mu - 1) \mu^0 \right],
\]
with

\[ r_m = Z_S^{-1} r_{S_0}, \quad r_\mu = Z_P^{-1} r_{P_0}. \] (4.19)

Here, the ratios \( r_m, r_\mu \) are finite functions of the gauge coupling, which can in principle be determined by axial Ward identities in the chiral limit. A few comments are in order, in relation to the practical considerations made in subsect. 4.1:

- The above counterterm structure applies to the complete theory with \( N_f = 4 \) dynamical quarks, for which our preferred choice of twist angles is \( \alpha = \pi/2 \) and \( \beta = 0 \) (partial twist). The latter condition translates to renormalised twisted parameters

\[ \mu_{R,s} = \mu_{R,c} = 0, \] (4.20)

which is achieved by setting

\[ \mu_s = \mu_c = 0. \] (4.21)

Due to \( \mu_u = -\mu_d = \mu_l \), this implies \( \mu^0 = 0 \) and thus no flavour mixing in the twisted mass renormalisation pattern expressed by eq. (4.18). On the other hand, the condition concerning the twist angle \( \alpha \) translates into

\[ m_{R,l} = 0, \] (4.22)

which, due to eq. (4.17) implies that the bare mass of the light quarks must be tuned as follows,

\[ m_l = m_{cr} + \frac{(1 - r_m)}{2(1 + r_m)} (m_s + m_c - 2m_{cr}), \] (4.23)

i.e. there is an offset of \( O(1) \) to the linear divergence cancelled by \( m_{cr} \).

- The ratios \( r_m \) and \( r_\mu \) depend implicitly on the number of dynamical quark flavours. In particular, their quenched values are \( r_m = r_\mu = 1 \), i.e. the flavour mixing terms in eqs. (4.17) and (4.18) are absent in this case \([36]\). Hence, the fully twisted cases \( \alpha = \pm \beta = \pi/2 \) are obtained by just setting all standard bare masses equal to the critical mass \( m_{cr} \).

- In the partially quenched case it is obvious that valence quark masses do not participate in the renormalisation of other quark flavours. More specifically, for the case of interest with \( N_f = 2 \) light dynamical flavours, the mass renormalisation pattern reduces to

\[ m_{R,l} = Z_S^{-1} r_m (m_l - m_{cr}), \] (4.24)

\[ m_{R,s,c} = Z_S^{-1} [m_{s,c} - m_{cr} + (r_m - 1) (m_l - m_{cr})], \] (4.25)

\[ \mu_{R,i} = Z_P^{-1} \mu_i. \] (4.26)
This implies that the fully twisted case, $\alpha = \pm \beta = \pi/2$, requires a quenched-like tuning $m_l = m_s = m_c = m_{\text{cr}}$, while for the partially twisted case, $\alpha = \pi/2, \beta = 0$, the requirement is $m_l = m_{\text{cr}}$ and $\mu_s = \mu_c = 0$.

### 4.2.3 Determination of the twist angles $\alpha$ and $\beta$

In practice, the twist angles are defined by ratios of the renormalised quark masses appearing in the renormalised PCAC and PCVC relations. In general, one therefore needs to discuss the renormalisation of the currents and densities which appear in the PCAC and PCVC relations. If we restrict attention to flavour off-diagonal quark bilinear operators ($i \neq j$), the symmetries imply a multiplicative renormalisation in all cases,

$$\begin{align*}
(A_R)_{\mu,ij} &= Z_A A_{\mu,ij}, \\
(V_R)_{\mu,ij} &= Z_V V_{\mu,ij}, \\
(P_R)_{ij} &= Z_P P_{ij}, \\
(S_R)_{ij} &= Z_S S_{ij},
\end{align*}$$

where the bare fields are defined as in the classical continuum theory, eq. (3.14). It is well-known that the scale independent renormalisation constants $Z_A$ and $Z_V$ as well as the ratio $Z_P/Z_S$ can be determined by imposing axial Ward identities as normalisation conditions. To obtain the scale-dependent renormalisation constants $Z_P$ or $Z_S$, it is then sufficient to impose a further quark mass independent renormalisation condition on one of the densities. The choice is largely arbitrary and does not affect the determination of the twist angles as the renormalisation constant cancels in quark mass ratios. Given the renormalised quark bilinear fields, and a choice of bare parameters, the 6 renormalised mass parameters (2 for the mass degenerate light quarks and 4 for strange and charm quarks) can be obtained by solving a system of 6 independent equations, which follow from the renormalised PCAC and PCVC relations for different flavour combinations.

Fortunately the situation is much simpler in the cases of practical interest, namely the choices $\alpha = \pm \beta = \pi/2$ and $(\alpha, \beta) = (\pi/2, 0)$, which we now discuss in more detail:

- To obtain $\alpha = \pm \beta = \pi/2$ all renormalised standard quark masses should vanish, $m_{R,l} = m_{R,s} = m_{R,c} = 0$, which implies that all bare standard quark masses are equal. The corresponding critical bare mass parameter $m_{\text{cr}}$ can be obtained by requiring

$$\partial_\mu A_{\mu,\bar{u}d} = 0,$$

for some correlation function of the axial current. Note that the renormalisation constant $Z_A$ is not needed here, and the angles $\alpha = \pi/2$ and $\beta = \pm \pi/2$ are now fixed up to a sign, which is determined by the sign of the bare twisted mass parameters. Moreover, the fully twisted cases are special because the values of

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Footnote 7: The determination of $Z_V$ could be avoided by using the point split vector current which follows from the exact flavour symmetry of mass degenerate standard Wilson quarks.
the renormalised twisted masses are not needed for the definition of the twist angles.

- The choice $\beta = 0$ is easily realised by just setting $\mu_s = \mu_c = 0$, as the counterterm structure then implies $\mu_{R,s} = \mu_{R,c} = 0$. Setting the twist angle $\alpha = \pi/2$ is then still achieved by requiring (4.28). However, the counterterm structure (4.23) implies that this determination of $m_l$ must be repeated every time the parameters $m_s$ and $m_c$ are changed.

Finally we remark that the definition of renormalised quark masses through the PCAC and PCVC relations is convenient, as it can be applied both in the (partially) quenched and in the full theory. In this way one may bypass the discussion of the quark mass counterterms in the partially quenched case.

### 4.3 Renormalisation pattern of $O_{VA+AV}^\pm$

In view of the $\Delta I = 1/2$ amplitudes, we are interested in the counterterm structure of the operator $O_{VA+AV}^\pm$ in the presence of twisted mass terms. We apply again a spurion analysis. In particular, the flavour structure of the operator suggests to consider the two flavour exchange symmetries

\begin{align}
  d \leftrightarrow s, & \quad m_d \leftrightarrow m_s, \quad \mu_d \leftrightarrow \mu_s, \\
  u \leftrightarrow c, & \quad m_u \leftrightarrow m_c, \quad \mu_u \leftrightarrow \mu_c,
\end{align}

combined with charge conjugation and spurionic parity discussed in sect. 4.2.1. Power counting and the behaviour under these symmetry transformations imply the following renormalisation pattern:

\begin{align}
  (O_R)^\pm_{VA+AV} &= Z^\pm \{ O_{VA+AV}^\pm + c^\pm_P P_{sd} + c^\pm_S S_{sd} \}. 
\end{align}

Note that, compared to standard Wilson quarks, the only change consists in the addition of the scalar density. The symmetries also determine the behaviour of the coefficients in the small $a$ expansion. For the leading terms we find:

\begin{align}
  c^\pm_P &= \frac{1}{a} \left\{ (m_c - m_u)(m_s - m_d) c^\pm_{P,a} + (\mu_c - \mu_u)(\mu_s - \mu_d) c^\pm_{P,b} \right\} + O(1), \\
  c^\pm_S &= \frac{1}{a} \left\{ (m_c - m_u)(m_s - m_d) c^\pm_{S,a} + (\mu_c - \mu_u)(m_s - m_d) c^\pm_{S,b} \right\} + O(1),
\end{align}

where the coefficients on the r.h.s. are functions of the bare coupling only. We observe that both coefficients $c^\pm_{P,S}$ are linearly divergent in general. Simplifications occur in special cases: if down and strange quarks are taken to be mass degenerate, $m_s = m_d$, \(20\)
\(\mu_s = \mu_d\), then both coefficients vanish identically due to the exact symmetry under a charge conjugation combined with the flavour exchange symmetry, \(s \leftrightarrow d\). Another important simplification occurs in the fully twisted cases discussed above, since

\[
m_u = m_d = m_s = m_c \Rightarrow c_S^\pm = O(1),
\]

so that one is left with the linear divergence in \(c_P^\pm\), which takes the form

\[
c_P^\pm = \frac{1}{a} (\mu_c - \mu_u)(\mu_s - \mu_d)c_{P,b}^\pm + O(a),
\]

i.e. subleading terms of O(1) are found to be absent.

### 4.4 O(\(a\)) improved action for fully twisted quarks

While systematic O(\(a\)) improvement of matrix elements of four-quark operators is beyond the scope of this paper, the discussion of the fully twisted case in section 5 shows that some simplifications occur if the action is O(\(a\)) improved. To investigate the structure of the O(\(a\)) counterterms in the special case of the fully twisted tmQCD action, we make use of results of ref. [38], which were obtained for two-flavour tmQCD with degenerate quarks. These results are directly relevant here, since, as discussed in subsection 4.1, a full twist of all quarks is implemented either in the quenched approximation or in the partially quenched case with dynamical (and mass degenerate) up and down quarks.

In the following it is assumed that the massless theory has been O(\(a\)) improved by the addition of the Sheikholeslami-Wohlert term to the action and of the counterterm proportional to \(c_A\) to the axial current [33]. Let us now suppose that the fully twisted case has been realised by tuning the standard bare masses to their critical value as explained in subsection 4.2.3. The O(\(a\)) effects in the renormalised light mass parameters can then be inferred from the result of ref. [38], as the quenched strange and charm quarks may not generate any additional counterterms:

\[
m_{R,i} = Z_{S_i}^{-1} \tilde{b}_m a\mu_l^2 + O(a^2),
\]

\[
\mu_{R,i} = Z_p^{-1} \mu_l + O(a^2).
\]

To find the counterterm structure for the strange and charm mass parameters, we use the fact that both quarks remain in the quenched approximation. Hence, one may imagine that either quark is a member of a mass degenerate quark doublet, with partners that do not enter any of the correlation functions, and are therefore completely decoupled from the theory. The renormalisation for each doublet then proceeds independently with the result (\(i = s, c\)),

\[
m_{R,i} = Z_{S_i}^{-1} \left\{ b_m a\mu_l^2 + \tilde{b}_m a\mu_l^2 \right\},
\]

\[
\mu_{R,i} = Z_p^{-1} \mu_i,
\]
where the new coefficients $\tilde{b}'_{m_i}$ are non-zero only if the light quarks are dynamical. At this point we recall that in the two flavour theory the set of $O(a)$ mass counterterms as determined by the lattice symmetries is over-complete [38]. More precisely, an axial rotation re-parameterises the mass counterterm basis, implying that there is a one-parameter family of equivalent $O(a)$ improved theories. This freedom may then be used to set one of the improvement coefficients to a fixed value. Hence, in the fully quenched case we may now choose to set

$$\tilde{b}_{ml} = \tilde{b}_{ms} = \tilde{b}_{mc} = 0,$$

and, as a result, all the renormalised quark mass parameters are $O(a)$ improved. In the partially quenched case we may set $\tilde{b}_{ml} = 0$, and for $i = s, c$,

$$\tilde{b}_{mi} = -\tilde{b}'_{mi} \mu_i^2 / \mu_i^2.$$  

(4.41)

We conclude that in the fully twisted cases, there is a choice for the $O(a)$ mass counterterms such that the action is $O(a)$ improved, provided that the action and the axial current have been $O(a)$ improved in the chiral limit.

5 $K \to \pi$ transitions from twisted mass lattice QCD

We now show how to extract $K^+ \to \pi^+$ matrix elements from tmQCD correlation functions. We will mostly be concerned with the determination of the additive counterterms to the renormalised operator, or with corresponding subtractions of its correlation functions. The multiplicative operator renormalisation can be performed using standard techniques [39,40,29,41] and does not pose any further conceptual problems.

In what follows we will refer to QCD with a standard parameterisation of the quark mass term as “standard QCD”, as opposed to QCD with a twisted mass term. Their respective renormalised correlation functions are thus related by a chiral rotation of the fields, according to the discussion in section 3.

5.1 From correlation functions to matrix elements

In standard QCD, the $K^+ \to \pi^+$ matrix elements can be obtained from the Euclidean 3-point function

$$G_{K\pi}^\pm(x, y, z) = \langle \varphi_\pi(x)(O_R)^\pm_{VV+AA}(y)\varphi_K(z) \rangle_{(0,0)},$$

(5.1)

where $\varphi_\pi$ and $\varphi_K$ are interpolating fields with the quantum numbers of the charged pion and kaon, respectively. Simple examples are the local fields,

$$\varphi_\pi(x) = P_{du}(x), \quad \varphi_K(z) = P_{us}(z),$$

(5.2)
but more complicated choices are possible and indeed often necessary to obtain a signal in numerical simulations. Based on the transfer matrix formalism, the spatial Fourier transform

\[ \tilde{G}_{K\pi}^{\pm}(x_0, z_0; p, q) = a^6 \sum_{x, z} e^{i(px - qz)}G_{K\pi}^{\pm}(x, 0, z) \]  \hspace{1cm} (5.3)

can then be shown to behave, for \( x_0 \to \infty \) and \( z_0 \to -\infty \), as

\[ \tilde{G}_{K\pi}^{\pm}(x_0, z_0; p, q) \sim Z_\pi Z_K \exp \left( -E_\pi(p)x_0 + E_K(q)z_0 \right) \times \langle \pi^+, p | (O_R)^{\pm}_{VV+AA}(0) | K^+, q \rangle. \]  \hspace{1cm} (5.4)

Here, neglected terms are exponentially suppressed contributions of higher intermediate states in either the pion or the kaon channel. The constants \( Z_\pi \) and \( Z_K \), as well as the pion and kaon energies \( E_\pi(p) \) and \( E_K(q) \) can be determined from the 2-point functions of the interpolating kaon and pion fields, so that one can isolate the desired matrix element of the renormalised operator. In fact the matrix element itself is used to completely specify the renormalised operator, by imposing the condition

\[ \langle \pi^+, 0 | (O_R)^{\pm}_{VV+AA}(0) | K^+, 0 \rangle = 0. \]  \hspace{1cm} (5.5)

Note that, even with a chirally invariant regularisation, such a condition may be used in order to determine the O(1) subtraction coefficients \( c^\pm \) in eq. (2.27).\(^8\) This arbitrariness is closely related to the fact that the \( K \to \pi \) matrix elements are not directly linked to a physical observable. Indeed, it is easy to see that the subtracted counterterm does not contribute to physical \( K \to \pi \pi \) amplitudes. This situation is reflected in chiral perturbation theory, where the condition (5.5) determines the unphysical coupling \( g_8' \).

It is actually convenient to impose the renormalisation condition (5.5), as it facilitates the matching to chiral perturbation theory.

### 5.2 Renormalised correlation function in tmQCD

In the twisted mass QCD framework, we expect that the properly renormalised correlation functions are mapped onto their standard QCD counterpart in the same way as in the classical continuum theory \[^{31}\]. According to Sect. 3 we can thus write

\[ G_{K\pi}(x, y, z) = \left\langle \bar{\psi}_\pi(x) \cos \left( \frac{\alpha + \beta}{2} \right) (O_R)^{\pm}_{VV+AA}(y) \right. \]

\[ \left. - i \sin \left( \frac{\alpha + \beta}{2} \right) (O_R)^{\pm}_{VA+AV}(y) \right\rangle \bar{\psi}_K(z) \rangle_{(\alpha, \beta)}, \]  \hspace{1cm} (5.6)

\(^8\)Instead of the above condition, in simulations with Ginsparg-Wilson quarks it is customary to determine the subtraction coefficient by imposing that the operator matrix element of the unphysical \( K \to 0 \) transition (with the \( K \)-meson at rest) vanishes.
where \( \tilde{\varphi}_\pi \) and \( \tilde{\varphi}_K \) denote the transformed source fields, which can be worked out once a specific choice of pseudoscalar sources \( \varphi_\pi \) and \( \varphi_K \) has been made. For instance, to reproduce the local source fields of eq. (5.2) up to terms of \( O(a) \), one defines

\[
\tilde{\varphi}_K = \cos \left( \frac{\alpha + \beta}{2} \right) (P_R)_{us} + i \sin \left( \frac{\alpha + \beta}{2} \right) (S_R)_{us}, \quad \tilde{\varphi}_\pi = (P_R)_{du}.
\] (5.7)

Note that for generic twist angles both parity components of \( O^\pm \) appear in the r.h.s. of eq. (5.6), while we would like to be left only with the operator \( O^\pm_{VA+AV} \), due to its nicer renormalisation properties. We therefore turn the tables and determine the physical interpretation of the tmQCD correlation functions with this operator alone:

\[
\langle \tilde{\varphi}_\pi(x)(O_R)^{\pm}_{VA+AV}(y)\tilde{\varphi}_K(z) \rangle_{(\alpha,\beta)} = \langle \varphi_\pi(x) \left[ \cos \left( \frac{\alpha + \beta}{2} \right) (O_R)^{\pm}_{VA+AV}(y) \right.
\]
\[
+ i \sin \left( \frac{\alpha + \beta}{2} \right) (O_R)^{\pm}_{VV+AA}(y) \left. \right] \tilde{\varphi}_K(z) \rangle_{(0,0)} = i \sin \left( \frac{\alpha + \beta}{2} \right) G^\pm_{K\pi}(x,y,z). \] (5.8)

Here, the last step is trivial in the fully twisted case, \( \alpha = \beta = \pi/2 \), for which the cosine in the first term on the r.h.s. vanishes. On the other hand, for generic values of the twist angles the cosine multiplies a standard QCD correlation function which vanishes by parity. Hence, by computing the l.h.s. of eq. (5.8) in twisted mass QCD one obtains the desired correlation function up to a known factor, and the \( K \to \pi \) matrix element is then obtained in the standard manner. It is important at this point, however, to stress that eq. (5.8) holds exactly only in the continuum limit, and assumes that physical parity, defined through eq. (3.10), is properly restored in renormalised tmQCD. In principle this can be achieved in two ways: given the twist angles, it may be possible to impose renormalisation conditions so that the renormalised composite fields assume the expected continuum behaviour under parity, up to cutoff effects. Alternatively, one may be able to identify the parity violating contributions to the correlation function on the l.h.s. of eq. (5.8), so that the parity conserving QCD correlator \( G^\pm_{K\pi} \) can be obtained. Moreover, this is only required in the asymptotic regime where the matrix element is extracted.

In practice, a combination of both methods seems advisable. Hence we begin by identifying three sources of parity violating contributions to the tmQCD correlation function in the l.h.s. of eq. (5.8):

(i) The operator \( O^\pm_{VA+AV} \) has linear divergences of either parity, cf. eq. (4.31).

(ii) In general, the interpolating fields \( \tilde{\varphi}_K, \tilde{\varphi}_\pi \) may break physical parity. However, once the twist angles \( \alpha, \beta \) are defined from the renormalised PCAC and PCVC relations, \( \tilde{\varphi}_K, \tilde{\varphi}_\pi \) may be chosen so that parity holds up to \( O(a) \) effects (explicit examples will be given in the following).
In general, the action will have parity breaking $O(a)$ counterterms. In the spirit of Symanzik’s effective continuum theory, these counterterms can be treated as operator insertions, and thus contribute at $O(a)$ to the correlation function.

As a consequence, unwanted $O(1)$ contributions which originate from parity violation may arise by combining the parity violating linear divergence of the four-quark operator with parity violating $O(a)$ terms from either the action or the interpolating fields. Hence, if the parity breaking linear divergence of the four-quark operator is subtracted by imposing an appropriate renormalisation condition, the parity violating contributions to the correlation function are $O(a)$.

In the following we make two specific choices for the twist angles $\alpha$ and $\beta$ (cf. subsect. 4.1). For both cases we explain in detail how to obtain the $K \to \pi$ matrix elements from the tmQCD correlation functions on the l.h.s. of eq. (5.8).

5.3 The fully twisted case $\alpha = \beta = \pi/2$

For simplicity we specify local source fields which, for $\alpha = \beta = \pi/2$ read

$$\tilde{\phi}_K = i(S_R)_{us}, \quad \tilde{\phi}_\pi = (P_R)_{du}. \quad (5.9)$$

We have already pointed out that the fully twisted case is special in that the operators of interest are directly matched to each other; thus the $K^+ \to \pi^+$ correlation function (5.1) simplifies to

$$G^+_{K\pi}(x,y,z) = \langle (P_R)_{du}(x)(O_R)_{VA+AV}^{\pm}(y)(S_R)_{us}(z) \rangle_{(\pi/2,\pi/2)}. \quad (5.10)$$

It follows that, up to cutoff effects, the renormalised four-quark operators have definite physical parity $P$, viz.

$$P[(O_R)_{VA+AV}^{\pm}] = +1. \quad (5.11)$$

On the other hand, for the dimension-3 counterterms we have

$$P[P_{sd}] = -1 \quad P[S_{sd}] = +1, \quad (5.12)$$

i.e. the linearly divergent coefficient $c_P^{\pm}$ multiplies a parity odd counterterm, while the finite counterterm proportional to $c_S^{\pm}$ is parity even. This implies that, out of the two renormalisation conditions required to determine the counterterm coefficients $c_P^{\pm}$ and $c_S^{\pm}$, the one determining $c_P^{\pm}$ must restore physical parity of the renormalised operator. For example, the condition

$$\langle (O_R)_{VA+AV}^{\pm}(x)(P_R)_{du}(y) \rangle_{(\pi/2,\pi/2)} = 0, \quad (5.13)$$

enforces parity conservation, as can be seen from its translation to standard QCD,

$$\langle i(O_R)_{VV+AA}^{\pm}(x)(P_R)_{du}(y) \rangle_{(0,0)} = 0. \quad (5.14)$$
In terms of the bare operators eq. (5.13) reads

\[ 0 = \langle O_{\Lambda+AV}^\pm(x) P_{ds}(y) \rangle_{(\pi/2,\pi/2)} \]
\[ + c_P^\pm \langle P_{sd}(x) P_{ds}(y) \rangle_{(\pi/2,\pi/2)} \]
\[ + c_S^\pm \langle S_{sd}(x) P_{ds}(y) \rangle_{(\pi/2,\pi/2)} . \]

(5.15)

Note that this equation indeed determines the coefficient \( c_P^\pm \), as the last term on the r.h.s. satisfies

\[ \langle S_{sd}(x) P_{ds}(y) \rangle_{(\pi/2,\pi/2)} = (Z_P Z_S)^{-1} \langle (S_R)_{sd}(x) (P_R)_{ds}(y) \rangle_{(0,0)} , \]

and thus vanishes by parity up to O(\( a \)). In particular, the prefactor \( c_S^\pm \), being of O(1), does not affect this conclusion.

We may now insert the renormalised operator \( (O_R)_{\Lambda+AV}^\pm \) (with \( c_P^\pm \) determined as above and \( c_S^\pm \) as yet undetermined) in the correlation function (5.10). As the mesonic source operators of eq. (5.9) are also parity eigenstates,

\[ \mathcal{P}[S_{us}] = -1 \quad \mathcal{P}[P_{du}] = -1 . \]

(5.17)

the remaining parity breaking effects in the correlation function (5.10) are at most of O(\( a \)), being combinations of O(\( a \)) effects from either the action or the mesonic source fields with an O(1) term of the four-quark operator. It thus remains to determine the finite counterterm proportional to \( c_S^\pm \). This can be done by imposing the condition (5.5) on the \( K^+ \to \pi^+ \) matrix element which, in the current tmQCD framework, is obtained from the correlation (5.10).

### 5.4 Sidestepping the power divergence

As explained in subsection 4.4, the action in the fully twisted cases can be considered O(\( a \)) improved, provided O(\( a \)) improvement has been correctly implemented in the massless theory. In this situation, the above renormalisation procedure can be further simplified, as the determination of the coefficient \( c_P^\pm \) from the condition (5.15) can be avoided.

To see this we write explicitly the correlation \( G_{K\pi}^\pm(x,y,z) \) in tmQCD:

\[ G_{K\pi}^\pm(x,y,z) = Z_P Z_S Z \left[ (P_{du}(x) O_{\Lambda+AV}^\pm(y) S_{us}(z))_{(\pi/2,\pi/2)} \right] \]
\[ + c_P^\pm \langle P_{du}(x) P_{sd}(y) S_{us}(z) \rangle_{(\pi/2,\pi/2)} \]
\[ + c_S^\pm \langle P_{du}(x) S_{sd}(y) S_{us}(z) \rangle_{(\pi/2,\pi/2)} \]  

(5.18)
and examine in detail the correlation proportional to $c^\pm_P$ on the r.h.s.. The operator product $P_{du}P_{sd}S_{us}$ is an odd parity eigenstate, giving vanishing $O(1)$ contributions. The $O(a)$ corrections (which give rise to $O(1)$ contributions to the original correlation function $G_{K\pi}^\pm$) may arise from three sources, as listed in subsect. 5.2:

(i) The parity-even $O(a)$ correction to the operator insertion $P_{sd}$ has the form $a(\mu_s + \mu_d)S_{sd}$, due to the symmetries of the lattice action. This term amounts to a re-definition of $c^\pm_S$ and can thus be ignored.

(ii) The even parity $O(a)$ corrections to the kaon source $S_{us}$ are proportional to $(\mu_u + \mu_s)P_{us}$, while the analogous counterterm for the pion only appears at $O(a^2)$ (for mass degenerate light quarks); the $O(a)$ correction to the Fourier transformed correlation function is then given by

$$a^6 \sum_{x,z} e^{i(px-qz)} \langle P_{du}(x)P_{sd}(0)P_{us}(z) \rangle_{(\pi/2,\pi/2)} \to_{z_0 \to -\infty} e^{z_0 E_{K^S}(q)}, \quad (5.19)$$

where we have exhibited the expected asymptotic factor for large negative $z_0$, and $K^S$ denotes the lowest scalar excitations in the kaon channel. It is not clear what the exact nature of this state is. Candidates are one-particle states with the opposite parity, or multi-particle states. For instance, a $J = 0$ two-particle state consisting of a kaon and a neutral pion shares all the lattice symmetries with the kaon, and might therefore be the next lightest state with opposite physical parity. In any case, we expect the energies of the excited states to be much higher than the kaon energies themselves. Therefore, in the asymptotic regime, the relative suppression factor $\exp\{z_0 [E_{K^S}(q) - E_{K}(q)]\}$ of the second term on the rhs of eq. (5.18) should be significant.

(iii) Finally, as the $O(a)$ contribution of the action vanishes with the appropriate choice of the counterterm basis (cf. subsect. 4.4), the action contributes at most to $O(a^2)$. This combines with the linear divergence of the operator to yield an $O(a)$ effect to $G_{K\pi}^\pm$. Here it is crucial that the action be $O(a)$ improved, as the insertion of action counterterms into the correlation function comes with a space-time integration, which makes the effect non-local. In particular, it would not be possible to argue in terms of the asymptotic regime of the correlation function as we did in (ii) with the localised counterterms to the kaon source field.

We conclude that in the fully twisted case the $c^\pm_P$ term in eq. (5.18) need not be subtracted explicitly, as it leads at most to $O(1)$ contributions to $G_{K\pi}^\pm$ which are exponentially suppressed, due to the energy gap between scalar and pseudoscalar sector. Remarkably, the only subtraction to be carried out explicitly is the finite, parity conserving counterterm proportional to $c^\pm_S$. One is thus left with a renormalisation
structure that closely resembles the one found in regularisations that preserve chiral symmetry.

### 5.5 The partially twisted case with \( \beta = 0 \)

In this case, the operator \( O_{VA+AV}^\pm \) is mapped to a linear combination of parity odd and parity even pieces (cf. eq. [5.25]). Therefore, it is not clear how to impose a parity restoration condition for the operator. We therefore proceed in two steps: first we subtract the two power divergent counterterms with some arbitrary prescription, e.g. by imposing the conditions

\[
\langle (\bar{O})_{VA+AV}^\pm (x)(P)_{ds}(y) \rangle_{(\pi/2,0)} = 0, \quad (5.20)
\]
\[
\langle (\bar{O})_{VA+AV}^\pm (x)(S)_{ds}(y) \rangle_{(\pi/2,0)} = 0. \quad (5.21)
\]

Here \( \bar{O}_{VA+AV}^\pm \) is the subtracted bare operator,

\[
\bar{O}_{VA+AV}^\pm = O_{VA+AV}^\pm + \bar{c}_{P}^\pm P_{sd} + \bar{c}_{S}^\pm S_{sd} \quad (5.22)
\]

and the coefficients \( \bar{c}_{P,S}^\pm \) are determined by eqs. [5.20,5.21]. This bare operator is only logarithmically divergent, and its renormalised counterpart is obtained by multiplicative rescaling with the usual renormalisation constant,

\[
(\bar{O}_{R})_{VA+AV}^\pm = Z_{R}^\pm \bar{O}_{VA+AV}^\pm. \quad (5.23)
\]

However, such a renormalised operator does not have the physical parity properties that ensure the restoration of parity in the continuum limit. Rather, a correctly renormalised operator will be of the form

\[
(OR)_{VA+AV}^\pm = Z_{R}^\pm \{ \bar{O}_{VA+AV}^\pm + \Delta_{c_{P}}^\pm P_{sd} + \Delta_{c_{S}}^\pm S_{sd} \}, \quad (5.24)
\]

with still unknown, but finite coefficients \( \Delta_{c_{P,S}}^\pm \). These should be determined so that the hadronic matrix element of the renormalised operator does not contain unwanted contributions of the wrong physical parity. This does not necessarily determine the renormalised operator itself. Indeed, it turns out that only a single coefficient needs to be determined, the other giving rise to contributions which are either of \( O(a) \) or exponentially suppressed or both, depending on the choice of interpolating kaon and pion fields.

To see this more explicitly, we have a closer look at the additive counterterms, \( P_{sd} \) and \( S_{sd} \). It is convenient to split both fields in pieces which are either even or odd under the physical parity transformation.

\[
P_{ds} = (P_{ds})_{\text{even}} + (P_{ds})_{\text{odd}}, \quad S_{ds} = (S_{ds})_{\text{even}} + (S_{ds})_{\text{odd}}. \quad (5.25)
\]
From the correspondence between the renormalised fields in tmQCD and standard QCD (cf. subsection 3.2) one then infers the explicit expressions,

\[(P_{ds})_{\text{even}} = \sin^2 \left( \frac{\alpha}{2} \right) P_{ds} + Z_S/Z_P \frac{i}{2} \sin(\alpha) S_{ds}, \quad (5.26)\]
\[(P_{ds})_{\text{odd}} = \cos^2 \left( \frac{\alpha}{2} \right) P_{ds} - Z_S/Z_P \frac{i}{2} \sin(\alpha) S_{ds}, \quad (5.27)\]
\[(S_{ds})_{\text{even}} = \cos^2 \left( \frac{\alpha}{2} \right) S_{ds} - Z_P/Z_S \frac{i}{2} \sin(\alpha) P_{ds}, \quad (5.28)\]
\[(S_{ds})_{\text{odd}} = \sin^2 \left( \frac{\alpha}{2} \right) S_{ds} + Z_P/Z_S \frac{i}{2} \sin(\alpha) P_{ds}, \quad (5.29)\]

where terms of O(\(a\)) have been neglected. To discuss contributions to the correlation function from which \(K^+ \to \pi^+\) matrix elements are extracted we first assume that the pion and kaon source fields have been chosen with definite physical parity, i.e. up to cutoff effects they generate excitations with only pion or kaon quantum numbers and thus of odd physical parity. It is then clear that the odd parity parts of the renormalised operator can only generate O(\(a\)) contributions to the correlation function. Neglecting these we are thus left with contributions of the parity even counterterms, i.e. only the combination,

\[\Delta c^+_{P} (P_{sd})_{\text{even}} + \Delta c^+_{S} (S_{sd})_{\text{even}}, \quad (5.30)\]

contributes at O(1). Moreover, as can be inferred from eqs. \((5.26, 5.28)\), the parity even operators are proportional to each other

\[(P_{ds})_{\text{even}} \propto (S_{ds})_{\text{even}}, \quad (5.31)\]

up to terms of O(\(a\)). This means that there is only a linear combination of counterterms which contribute at O(1), which can be written as

\[\left\{ \Delta c^+_{P} - Z_P/Z_S \frac{2i \cos^2(\alpha/2)}{\sin(\alpha)} \Delta c^+_{S} \right\} (P_{sd})_{\text{even}} \equiv d^+_{P} (P_{sd})_{\text{even}}. \quad (5.32)\]

Moreover, it is not necessary to determine the parity even part of \(P_{sd}\), as the corresponding parity odd part does only contribute at O(\(a\)). It is therefore enough to insert for the renormalised operator

\[(O_R)_{VA+AV}^+ \to Z^+ \{ \tilde{O}_{VA+AV}^+ + d^+_P P_{sd} \}. \quad (5.33)\]

In other words: for insertions into the \(K \to \pi\) correlation function with meson sources of definite parity, the replacement \((5.33)\) yields equivalent results up to O(\(a\)) effects. The remaining coefficient \(d^+_P\) is then determined non-perturbatively by the condition \((5.5)\) on the hadronic matrix element.

Finally, by the same arguments as in the preceding subsection we may relax the requirement that the meson sources have a definite parity. This is again due to the
expected energy gap between scalar and pseudoscalar channels, which implies an exponential suppression of the wrong parity contributions. The sources with a definite parity therefore just provide an additional suppression by a power of $a$ of these terms, which is not necessary for the extraction of the matrix element.

In conclusion, in the partially twisted case with $\beta = 0$, the two linearly divergent counterterms can be subtracted non-perturbatively by imposing two independent but otherwise arbitrary conditions on correlation functions involving the four-quark operator. Once this has been achieved it turns out that wrong parity contributions to the correlation function are of $O(a)$ provided that the mesonic source fields have odd parity. Otherwise they are in any case exponentially suppressed in the asymptotic regime where the matrix element is extracted. A remaining finite subtraction constant is determined in the usual way by the matrix element itself from eq. (5.5).

5.6 $K^0 \to \pi^0$ matrix elements

As stated earlier, the breaking of isospin symmetry in twisted mass lattice QCD obscures the decomposition of four-quark operators into $\Delta I = 1/2$ and $\Delta I = 3/2$ pieces. In order to obtain both effective couplings, $g_8$ and $g_{27}$, one may therefore opt to compute, besides the $K^+ \to \pi^+$ transition, also $K^0 \to \pi^0$ matrix elements.

The strategy used for $K^+ \to \pi^+$ matrix elements can be taken over virtually unchanged. However, a technical complication is generated by the fact that disconnected diagrams are now possible, as the self-contraction of the pion source does not vanish by flavour symmetry. Moreover, one may be worried about new power divergences, which may arise in the pion source field. For instance, the field

$$\tilde{\varphi}_{\pi^0} = \partial_{5} u - \partial_{5} d,$$

(5.34)

suffers from a quadratic divergence $\propto \mu_b/a^2$. However, we note that this can be easily bypassed with the choice of the axial current,

$$\tilde{\varphi}_{\pi^0} = A_3^0,$$

(5.35)

which, due to the $O(4)$ vector structure, does not suffer from additive renormalisation. Hence we conclude that, beyond possible practical problems relating to the quality of the signal in the numerical simulations, the $K^0 \to \pi^0$ matrix elements do not present any further theoretical challenge.

5.7 A comment on $K \to \pi\pi$ transitions

In principle, there is no obstacle to applying the strategies described here to the physical $K \to \pi\pi$ amplitudes. Parity is changed in this transition, so that only the parity odd operator contributes to the matrix element. This operator has nice renormalisation
properties already with standard Wilson quarks (2.28), so that the potential gain by using twisted mass QCD mainly consists in the elimination of unphysical zero modes.

A direct mapping of the operator $O_{\pm}^{VA+AV}$ in the twisted basis to the parity odd operator in the standard basis is obtained for twist angles $\alpha = -\beta = \pi/2$ [cf. eq. (3.28)]. Compared to the case of $\beta = \pi/2$ this implies that the sign of $\mu_s$ and $\mu_c$ are reversed. Alternatively, one may again set $\beta = 0$, and project on the desired matrix element by choosing interpolating fields for the two-pion and kaon states with the correct physical parity. However, a practical problem may arise from isospin symmetry breaking in lattice regularised tmQCD: for instance, the lattice symmetries do not distinguish the $I = 0$ two-pion state from the state with a single neutral pion. As the energy of a single pion is lower than the energy of the two-pion state, one needs to carry out a multi-state analysis which renders this approach more complicated. Nevertheless, the good news remains that unphysical zero modes can be eliminated whilst the renormalisation properties are no worse than in standard lattice QCD with Wilson type quarks.

6 Conclusions

Twisted mass lattice QCD provides a viable framework for a determination of $g_8$ and $g_{27}$, by allowing for comparatively cheap numerical computations of $K \rightarrow \pi$ matrix elements at light meson masses. In order to facilitate future practical implementations of this strategy, we summarise our results in the form of a recipe:

(i) Choose the number of dynamical quarks to be 0, 2, 3 or 4, with mass degenerate up and down quarks; the recommended twist angles are then $(\alpha, \beta) = (\pi/2, \pi/2)$ or $(\alpha, \beta) = (\pi/2, 0)$. The latter choice avoids a complex quark determinant if more than 2 quarks are dynamical.

(ii) Translate the twist angles to bare mass parameters: $(\alpha, \beta) = (\pi/2, \pi/2)$ means that all standard mass parameters are tuned to the critical mass $m_{cr}$, which can be obtained from the PCAC relation as usual. The physical quark masses are then determined by the twisted mass parameters $\mu_l, \mu_s, \mu_c$ which are fixed by matching appropriate experimental quantities.

The second option, $(\pi/2, 0)$, corresponds to $\mu_s = \mu_c = 0$. For given mass parameters $m_s, m_c$, one then needs to determine $m_l$ so that the axial current in the light quark sector is conserved. A simplification occurs with quenched strange and charm quarks, where this is equivalent to setting $m_l = m_{cr}$, independently of $m_s, m_c$. The physical quark masses are determined in terms of $\mu_l, m_s$ and $m_c$.

(iii) Choose your preferred mesonic source fields for the kaon and pion; these need not be of definite physical parity, however, they should have a sufficiently large
overlap with the physical kaon or pion state. In the case of full twist, \((\pi/2, \pi/2)\), there are two ways to proceed:

- if \(O(a)\) improvement of the massless action and the axial current is implemented via the counterterms \(\propto c_{sw}\) and \(\propto c_A\) respectively, the tmQCD action can be considered \(O(a)\) improved and the linear divergence in the four-quark operator need not be subtracted. Just compute the bare 3-point function and the pion and kaon propagators, and go to the asymptotic regime to obtain the matrix element up to \(O(a)\) effects. Requiring the matrix element to vanish at zero meson momenta fixes the coefficient \(c_S^\pm\) of the finite counterterm.

- if \(O(a)\) improvement is not implemented, one needs to first determine \(c_P^\pm\) e.g. by imposing the parity restoration condition (5.13). Using the resulting subtracted operator one may proceed exactly as above.

In the case of partial twist, \((\pi/2, 0)\), one first subtracts the linear divergences by imposing two arbitrary renormalisation conditions such as (5.20, 5.21). Then one proceeds as above, using the subtracted operator. To fix the finite counterterm through the \(K \to \pi\) matrix element at vanishing meson momenta, one may use the substitution (5.33) which avoids determining the parity even part of the counterterm.

(iv) Repeat the calculation for a sequence of lattice spacings, keeping the physical scales fixed, and extrapolate to the continuum limit. Note that there exist various alternative strategies to compute the same matrix element. By varying the choice of twist angles, the way in which the linear divergences are subtracted, or the choice of mesonic source fields, one should obtain always the same matrix element up to \(O(a)\) effects. Thus, one may hope to improve the control of the continuum limit by pursuing a couple of alternative strategies in parallel.

(v) The continuum results obtained for various meson momenta and energies should be well described by leading order chiral perturbation theory, provided the meson masses and momenta are small enough. If so, the \(K^+ \to \pi^+\) matrix element allows to determine the linear combination \(\frac{2}{3}g_{27} + g_8\), while the matrix element for neutral mesons yields \(g_{27} - g_8\) (cf. subsect. 2.3). If the \(\Delta I = 1/2\) rule can be explained within QCD, one would expect the lattice results to reproduce the hierarchy \(g_8 \gg g_{27}\) obtained for the phenomenological estimates (2.18).

The strategy described above offers major improvements over previous attempts to compute \(K \to \pi\) transitions with Wilson-type quarks. Nevertheless, it is conceivable that further theoretical developments, along the lines of refs. 42,35, may lead to interesting variations and/or alternatives to the current work.
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