Twisted-mass lattice QCD with mass non-degenerate quarks

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The maximally twisted lattice QCD action of an $SU_f(2)$ doublet of mass degenerate Wilson quarks gives rise to a real positive fermion determinant and it is invariant under the product of standard parity times the change of sign of the coefficient of the Wilson term. The existence of this spurionic symmetry implies that $O(a)$ improvement is either automatic or achieved through simple linear combinations of quantities taken with opposite external three-momenta. We show that in the case of maximal twist all these nice results can be extended to the more interesting case of a mass non-degenerate quark pair.

1. Introduction

It has been shown in ref. \cite{1} that in lattice QCD (LQCD) with mass degenerate $SU_f(2)$ doublets of Wilson fermions it is possible to improve the approach to the continuum limit of correlation functions of gauge invariant multiplicative renormalizable (m.r.) operators by taking the arithmetic average (Wilson average - WA) of pairs of correlators computed in theories regularized with Wilson terms of opposite sign and identical values of the subtracted (unrenormalized) lattice quark mass, $m_q^W = M_0 - M_{cr}$ with $M_0$ the bare quark mass. Equivalently one can take appropriate linear combinations of the correlators computed in a given regularization (fixed sign of the Wilson term) but with opposite values of $m_q^W$ (mass average - MA). Improved hadronic masses and matrix elements can be similarly obtained by taking WA’s of the corresponding quantities separately computed within the two regularizations.

To avoid the difficulties related to the nature of the spectrum of the Wilson–Dirac (WD) operator (here we are referring to the well-known problem of the existence of “exceptional configurations” \cite{23}) twisted-mass lattice QCD (tm-LQCD) \cite{4} should be used for the actual computation of the correlators taking part to the averages. The fermionic determinant of tm-LQCD is, in fact, real and positive on arbitrary gauge backgrounds, as long as the quark mass is non-vanishing. All the nice cancellations of $O(a)$ terms that one finds in the standard Wilson case extend to tm-LQCD with mass degenerate quark doublets.

Peculiar simplifications occur if the twisting angle is taken to be equal to $\pi/2$ (maximal twist). This choice is particularly useful for applications because essentially all interesting physical quantities (e.g. hadronic masses and matrix elements of m.r. operators between states with vanishing three-momenta) can be extracted from $O(a)$ improved lattice data without making recourse to any WA.

The main goal of this note is to show that in the maximally twisted case positivity of the determinant and $O(a)$ improvement without WA can be extended to encompass the more interesting situation in which mass non-degenerate quark pairs are considered. This is a preliminary, necessary step if one wants to set up a realistic computational scheme for operator matrix elements.

For future applications it is important to stress that the approach we propose is very flexible as it allows to regularize different flavours with dif-
ferently twisted Wilson terms. As discussed in
detail in [2], it is possible to exploit this freedom
in order to improve the chiral behaviour of lat-
tice correlators to the point of (hopefully) killing
all the unwanted “wrong chirality mixings” that
affect in the standard Wilson [6] and twisted-
mass [17] regularizations of QCD the construc-
tion of m.r. operators. Of special importance is
the application of this new strategy to the con-
struction of the m.r. operators which represent
the CP-conserving, \( \Delta S = 2 \) and \( \Delta S = 1 \) effective
weak Hamiltonian on the lattice.

The presentation of the material is divided in
two parts. In the first part (sect. 2) we spell out
in detail the formulae relevant for mass degen-
erate quark pairs with the choice \( \pm \pi/2 \) (maxi-
mal twist) for the twisting angle. In the second
part (sect. 3) we discuss how one can deal with
mass non-degenerate pairs of quarks without los-
ing \( O(a) \) improvement, or the positivity of the
fermion determinant. The latter property, which
is obvious in the case of mass degenerate dou-
blets, is crucial for being able to actually carry
out numerical Monte Carlo simulations. Conclu-
sions can be found in sect. 4. In Appendix A
we prove the renormalizability of the maximally
twisted fermion action both in the case of mass
degenerate and mass non-degenerate quarks. The
proof of the positivity of the fermion determinant
in the non-trivial case of mass non-degenerate
quarks is given in Appendix B.

2. A summary of tm-LQCD @ \( \pm \pi/2 \)

The twisted-mass lattice action of an \( SU_f(2) \)
flavour doublet of mass degenerate quark has the
form

\[
S_{F,D}^{(\omega)}[\psi, \bar{\psi}, U] = a^4 \sum_x \bar{\psi}(x) \left[ \gamma \cdot \nabla + \right. \\
+ e^{-i\omega \gamma_5 \tau_3} W_{cr}(r) + m_q \left. \right] \psi(x),
\]

where

\[
\gamma \cdot \nabla \equiv \frac{1}{2} \sum_{\mu} \gamma_{\mu} (\nabla_{\mu}^+ + \nabla_{\mu}),
\]

\[
W_{cr}(r) \equiv -a^2 \sum_{\mu} \nabla_{\mu}^+ \nabla_{\mu} + M_{cr}(r)
\]

and \( M_{cr}(r) = -M_{cr}(-r) \) is the critical quark
mass. We wrote the action in what is usually
called the “physical basis” [1], where \( m_q \), is taken
to be real (and positive) \(^2\). By undoing the twist-
ing of the Wilson term and bringing it fully to
the mass term, it was proved in ref. [11] that the
parameter \( M_{cr}(r) \) appearing in the action [11] is
equal to that of the corresponding standard Wil-
tson theory.

In this note we will concentrate on the maximal
twist case \( \omega = \pi/2 \), where eq. (1) becomes

\[
S_{F,D}^{(\pi/2)}[\psi, \bar{\psi}, U] = a^4 \sum_x \bar{\psi}(x) \left[ \gamma \cdot \nabla + \right. \\
- i\gamma_5 \tau_3 W_{cr}(r) + m_q \left. \right] \psi(x).
\]

The choices \( \omega = \pm \pi/2 \) are particularly useful be-
cause it can be proved [11] that, despite the fact
that the theory is not fully \( O(a) \) improved, can-
cellation of \( O(a) \) effects in quantities of physical
interest (like energies and operator matrix ele-
ments) is either automatic or obtainable with no
need of any WA. The proof of this statement
is sketched in sect. 2.2. \( O(a) \) ambiguities in the
knowledge of \( M_{cr}(r) \) do not spoil any of the above
results.

Furthermore it is important to observe that at
\( \omega = \pm \pi/2 \) the critical WD operator (i.e. the op-
erator in square parenthesis in eq. [11] with \( m_q = 0 \)
is anti-Hermitian, so its spectrum is purely imag-
inary. This means that the full WD operator
cannot have any vanishing eigenvalue as soon as
\( m_q \neq 0 \). This is also evident from the explicit
expression of its determinant, \( D_{F,D} \), which takes
the remarkably simple form

\[
D_{F,D} = \det \left[ Q_{cr}^T Q_{cr} + m_q^2 \right],
\]

where \( Q_{cr} = Q_{cr}^T \) is defined by eqs. [2] and [3].

While we can do for \( \omega = \pi/2 \) also holds for \( \omega = -\pi/2 \).

\(^2\)Unless differently stated, we employ here the notations
of ref. [1].

\(^3\)Whatever we say for \( \omega = \pi/2 \) also holds for \( \omega = -\pi/2 \).
present in (11), which one would need to include for renormalizability. Once $M_{A}(r)$ has been set to the appropriate value, the continuum limit is approached as usual by rescaling $g_{0}^{2}$ and $m_{q}$ according to the chosen renormalization conditions.

2.1. Non-singlet Ward-Takahashi identities

In this section we collect the expressions of the renormalized current and quark density operators entering the flavour non-singlet Ward-Takahashi identities (WTI’s) associated with the action (4). 

Renormalized vector and axial currents can be taken to be

\[
\begin{align*}
\hat{V}_{\mu}^{1} &= Z_{A} \bar{\psi} \gamma_{\mu} \frac{2}{2} \psi \\
\hat{V}_{\mu}^{2} &= Z_{A} \bar{\psi} \gamma_{\mu} \frac{2}{2} \psi \\
\hat{A}_{\mu}^{1} &= Z_{V} \bar{\psi} \gamma_{\mu} \gamma_{5} \frac{2}{2} \psi \\
\hat{A}_{\mu}^{2} &= Z_{V} \bar{\psi} \gamma_{\mu} \gamma_{5} \frac{2}{2} \psi
\end{align*}
\]

(6)

where to make contact with known quantities the (finite) renormalization constants, $Z_{V}$ and $Z_{A}$, introduced above are those for the local vector and axial currents of standard Wilson fermions, respectively. Notice the switch between identities (WTI’s) associated with the action (4).

With reference to eqs. (6), the non-singlet WTI’s with the insertion of the renormalized (multi-local) operator $\hat{O}(y)$ ($y \equiv \{y_{i}, i = 1, \ldots, n\} \neq x$) take the expected form (b = 1, 2, 3)

\[
\langle \partial_{\mu} \hat{V}_{\alpha}^{b}(x) \hat{O}(y) \rangle_{(r,m_{q})} = O(a)
\]

(7)

\[
\left\langle \left[ \partial_{\mu} \hat{A}_{\alpha}^{b}(x) - 2 \bar{\hat{m}}_{q} \hat{P}^{b}(x) \right] \hat{O}(y) \right\rangle_{(r,m_{q})} = O(a)
\]

(8)

with

\[
\bar{m}_{q} = Z_{P}^{-1} m_{q}
\]

(9)

provided one defines, in terms of bare quantities, the renormalized pseudo-scalar operators, $\hat{P}^{b}$, to be

\[
\hat{P}^{b} = Z_{P} \bar{\psi} \gamma_{\mu} \gamma_{5} \psi \quad b = 1, 2
\]

(10)

\[
\hat{P}^{3} = Z_{S^{0}} \left[ \frac{\psi^{T_{3}}}{T_{3}} \gamma_{5} \psi + a^{-3} \rho_{P} (am_{q}) \mathbb{I} \right]
\]

(11)

In eq. (11) the dimensionless real coefficient, $\rho_{P}(am_{q})$, in front of the power divergent term admits a polynomial expansion in $am_{q}$. Similarly to $Z_{V}$ and $Z_{A}$, $Z_{P}$ and $Z_{S^{0}}$ are the (logarithmically divergent) renormalization constants of the non-singlet pseudo-scalar and singlet scalar quark density of the standard Wilson regularization, respectively.

For completeness we also give the expression of the renormalized singlet scalar quark density operator, $\hat{S}^{0}$. By standard symmetry and dimensionality arguments, one finds

\[
\hat{S}^{0} = Z_{P} \left[ \bar{\psi} \psi + a^{-2} m_{q} \rho_{S^{0}} (am_{q}) \mathbb{I} \right]
\]

(12)

where $\rho_{S^{0}}$ is a dimensionless real coefficient with an even polynomial dependence on $am_{q}$. This parity property follows from the invariance of the action (4) under the spurionic symmetry $\mathbb{P}_{1/2} \times (m_{q} \rightarrow -m_{q})$ (eq. (62)). Formula (12) is rather interesting because it shows that the chiral order parameter is only affected by an $m_{q}/a^{2}$ power divergence, analogously to what happens with Ginsparg-Wilson fermions.

The equations of this section can be obtained by specializing to the case $\omega_{r} = \omega = \pi/2$ the corresponding formulae of ref. [1]. A direct and practical method to deduce them is to proceed in the following way. One starts by rotating the fermionic fields in the action (11) so as to have the Wilson term in the standard form (i.e. with no factor $\gamma_{5} T_{3}$ in front of it). At this point one can straightforwardly adapt to this instance the analysis of the structure of the mixing pattern of the chiral rotation of the Wilson term spelled out in detail in ref. [6] (see also ref. [6]). In a mass independent renormalization scheme renormalization constants can be computed in the massless limit ($m_{q} = 0$). For this reason it seemed to us a natural choice to keep for them the names they would have in the standard Wilson regularization. The final step of this method requires to rotate all the quark fields back into the physical basis we started from.

2.2. $O(a)$ improvement

It was proved in ref. [1] that the invariance of the action (4) under

\[
\mathcal{R}^{3}_{5} = \mathcal{R}_{5} \times (r \rightarrow -r) \times (m_{q} \rightarrow -m_{q}),
\]

(13)
\[ \mathcal{R}_5 \times \mathcal{D}_d, \]  
with \( \mathcal{R}_5 \) and \( \mathcal{D}_d \) defined in eqs. 164 and 165, respectively, implies the validity of the formula

\[
\langle O \rangle_{(m_q)}^{(\omega)WA} \equiv \frac{1}{2} \left[ \langle O \rangle_{(r,m_q)}^{(\omega)} + \langle O \rangle_{(-r,m_q)}^{(\omega)} \right] = \zeta^B_\omega(\omega,r) \langle O \rangle_{(m_q)}^{\text{cont}} + O(a^2),
\]

where \( O \) is any gauge invariant m.r. (multi-local) operator.

From 115 one can prove a number of physically interesting improvement formulae. To see this let us introduce the eigenstates \( |h,n,k\rangle_{(r,m_q)}^{(\omega)} \) (\( h \) and \( k \) represent the set of quantum numbers and three-momenta characterizing the state and \( n \) the excitation level) of the transfer matrix, \( \hat{T}(\omega,r,m_q) \), with eigenvalues \( E_{h,n}(k;\omega,r,m_q) \). The eigenvalue equation reads

\[
\hat{T}(\omega,r,m_q)|h,n,k\rangle_{(r,m_q)}^{(\omega)} = e^{-aE_{h,n}(k;\omega,r,m_q)}|h,n,k\rangle_{(r,m_q)}^{(\omega)}. \tag{16}\]

The notations of ref. 11 one gets the formulae

\[
E_{h,n}(k;\omega,r,m_q) + E_{h,n}(k;\omega,-r,m_q) = 2E_{h,n}(k;m_q) + O(a^2), \tag{17}\]

where \( B \) is a gauge invariant m.r. local operator. It is important to remark that in the whole argument about \( O(a) \) improvement of \( WA \)'s the twisting angle \( \omega \) is a totally inert label.

The interesting observation is that at \( \omega = \pi/2 \) the second term of the \( WA \)’s in eqs. 177 and 188, i.e. the quantities evaluated with Wilson parameter \(-r\), can be rewritten in terms of closely related quantities but evaluated with the value \( r \) of the Wilson parameter. As a consequence, \( O(a) \) improved estimates of energies and matrix elements can be obtained without having to average results from simulations with lattice actions differing by the sign of the Wilson term and critical mass.

Before coming to the proof of this statement, we recall from ref. 11 that at generic values of \( \omega \) the product

\[
P \times (\omega \rightarrow -\omega), \tag{19}\]

where \( P \) is the physical parity operator (\( x_P = (-x,t) \))

\[
P = \left\{ \begin{array}{ll}
U_0(x) & \rightarrow U_0(x_P), \\
U_k(x) & \rightarrow U_k^\dagger(x_P - a\hat{k}), \quad k = 1,2,3 \\
\psi(x) & \rightarrow \gamma_0\psi(x_P) \\
\bar{\psi}(x) & \rightarrow \bar{\psi}(x_P)\gamma_0
\end{array} \right.
\]

is a spurionic symmetry of the tm-LQCD action 11. Since \( [P \times (\omega \rightarrow -\omega)]^2 = \mathbb{1} \), (multi-local) m.r. operators can always be taken to have a definite parity, which can be read off from the formula

\[
\langle O^{(p)}(\{x_i\}) \rangle_{(r,m_q)}^{(\omega)} = (-1)^p \langle O^{(p)}(\{x_i\}) \rangle_{(r,m_q)}^{(-\omega)}. \tag{20}\]

This relation entails the possibility of defining a notion of parity for the eigenstates of the transfer matrix 11. One can, in fact, prove the validity of the following equations

\[
\hat{P}\hat{T}(\omega,r,m_q)\hat{P} = \hat{T}(-\omega,r,m_q), \tag{21}\]

\[
\hat{P}|h,n,k\rangle_{(r,m_q)}^{(\omega)} = \eta_{h,n}|h,n,-k\rangle_{(r,m_q)}^{(-\omega)}, \tag{22}\]

\[
E_{h,n}(k;\omega,r,m_q) = E_{h,n}(-k;\omega,-r,m_q), \tag{23}\]

where \( \hat{P} \) is the representative of the parity operation on the Hilbert space of states of the theory and \( \eta_{h,n} (\eta_{h,n}^2 = 1) \) is what we will call the parity of the state \( |h,n,k\rangle_{(r,m_q)}^{(\omega)} \). Indeed \( \eta_{h,n} \) can be taken to be an \( \omega \)-independent integer coinciding with the physical parity label of the corresponding continuum state. For details we refer the reader to Appendix F of ref. 11.

It is also immediate to recognize that the action 11 goes into itself under the transformation (we recall that \( \omega \) is defined mod \( 2\pi \))

\[
(r \rightarrow -r) \times (\omega \rightarrow \omega \pm \pi). \tag{24}\]
If in particular we set, say, \( \omega = \pi/2 \), the tm-LQCD action takes the form \( \mathbf{14} \) and the invariance \( \mathbf{24} \) becomes

\[
(r \rightarrow -r) \times (\omega \rightarrow -\omega) \big|_{\omega = \pi/2}.
\]

Either by inspection or by observing that, owing to \( \mathbf{24} \), \( \mathbf{19} \) is equivalent to

\[
P \times (r \rightarrow -r),
\]

we conclude that the action \( \mathbf{14} \) is invariant under \( \mathbf{26} \). This means that at \( \omega = \pi/2 \) eq. \( \mathbf{16} \) and equations from \( \mathbf{24} \) to \( \mathbf{28} \) can be rewritten in the form (for short we drop the twisting angle label)

\[
\left[ \hat{T}(r, m_q) - e^{-aE_h,n(k;r,m_q)} \right] \langle h, n, k \rangle = 0
\]

\( \mathbf{20} \)

\[
\hat{P} \hat{T}(r, m_q) \hat{P} = \hat{T}(-r, m_q), \quad \mathbf{28}
\]

\[
\hat{P} \langle h, n, k \rangle \big|_{(r, m_q)} = \eta_{h,n} \langle h, n, -k \rangle \big|_{(-r, m_q)}, \quad \mathbf{29}
\]

\[
E_{h,n}(k; r, m_q) = E_{h,n}(-k; -r, m_q). \quad \mathbf{30}
\]

Using the last two equations it is now possible to cast at \( \omega = \pi/2 \) the WA’s \( \mathbf{18} \) and \( \mathbf{17} \) in a form in which all the relevant lattice data are extracted from simulations carried out with the action \( \mathbf{14} \) and a given fixed value, \( r \), of the Wilson parameter. One gets, in fact, the formulae

\[
\langle h, n, k | B | h', n', k' \rangle \big|_{(r, m_q)} + \eta_B^{h,n,h',n',k,k'} \langle h, n, k | B | h', n', -k' \rangle \big|_{(r, m_q)} = 2\zeta_B(r) \langle h, n, k | B | h', n', k' \rangle \big|_{(m_q)} + O(a^2), \quad \mathbf{31}
\]

where \( \eta_B^{h,n,h',n',k,k'} = \eta_{h,n}(-1)\eta_{h',n'} \pm 1 \), and

\[
E_{h,n}(k; r, m_q) + E_{h,n}(-k; r, m_q) = 2E_{h,n}(k; m_q) + O(a^2).
\]

\( \mathbf{32} \)

Notice that in case the lattice matrix element \( \langle h, n, k | B | h', n', k' \rangle \big|_{(r, m_q)} \) is invariant under inversion of all the external three-momenta (like when all three-momenta vanish), the formula \( \mathbf{34} \) gets particularly simple. In fact, if \( \eta_B^{h,n,h',n',k,k'} = 1 \), the lattice matrix element turns out to be automatically \( O(a) \) improved, while if \( \eta_B^{h,n,h',n',k,k'} = -1 \) eq. \( \mathbf{31} \) implies that the \( O(a) \) improved estimate of \( \langle h, n, k | B | h', n', k' \rangle \big|_{(r, m_q)} \) is zero. This last result is in agreement with what one expects in the continuum limit from parity invariance.

An important instance of a quantity which is automatically \( O(a) \) improved is \( F_\pi \mathbf{1} \), as it can be extracted from two-point correlators evaluated at zero external three-momentum.

Eq. \( \mathbf{32} \) taken at \( k = 0 \) tells us that masses are automatically \( O(a) \) improved.

We end by observing that, although hadronic masses are automatically \( O(a) \) improved at \( \omega = \pm \pi/2 \), it is not possible to extract mass, from numerical simulations with a discretization error which is better than \( O(a) \) (unless the theory is fully \( O(a) \) improved à la Symanzik). The reason is precisely that at \( \omega = \pm \pi/2 \) the pion mass is automatically \( O(a) \) improved, even if the critical mass is known with an \( O(a) \) error (see Appendix D of ref. \( \mathbf{1} \)), thus it cannot be sensitive to \( O(a) \) discretization uncertainties in the critical mass. With an analogous argument a similar conclusion is reached if WTT’s are used to determine \( M_\pi \).

### 3. Mass non-degenerate quarks

The maximally twisted LQCD fermionic action of an \( SU_f(2) \) pair of mass non-degenerate quark can be conveniently written in the form

\[
S_{F,ND}^{(\pi/2)}[\psi, \bar{\psi}, U] = a^4 \sum_x \bar{\psi}(x) \left[ \gamma \cdot \nabla + \right. \quad \mathbf{33}
\]

\[
i\gamma_3 \tau_1 W_{\tau}(r) + m_q + \tau_3 \epsilon_q \bigg] \psi(x),
\]

where to keep the mass term real and flavour diagonal we have used the matrix \( \tau_3 \) to split the masses of the members of the doublet. Consequently the Wilson term was twisted with the flavour matrix \( \tau_1 \). Our notations are such that \( m_q \) and \( \epsilon_q \) are both positive.
What we said about the renormalizability of the fermion action in the mass degenerate case is valid also here and it is explicitly proved in Appendix A.

3.1. Non-singlet Ward-Takahashi identities

For mass non-degenerate quarks non-singlet WTI's take the continuum-like form \( x \neq y \)

\[
\langle \left[ \partial_\mu \hat{V}_\mu^1(x) - 2i\epsilon_q \hat{S}^2(x) \right] \hat{O}(y) \rangle_{(r, m_q, \epsilon_q)} = O(a)
\]

\[
\langle \left[ \partial_\mu \hat{V}_\mu^2(x) + 2i\epsilon_q \hat{S}^1(x) \right] \hat{O}(y) \rangle_{(r, m_q, \epsilon_q)} = O(a)
\]

\[
\langle \partial_\mu \hat{V}_\mu^3(x) \hat{O}(y) \rangle_{(r, m_q, \epsilon_q)} = O(a)
\]

if we make use of the definitions

\[
\hat{V}_\mu^1 = Z_V \bar{\psi} \gamma_\mu \frac{T_3}{2} \psi \quad \hat{V}_\mu^2 = Z_A \bar{\psi} \gamma_\mu \gamma_5 \frac{T_3}{2} \psi \quad \hat{V}_\mu^3 = Z_V \bar{\psi} \gamma_\mu \gamma_5 \frac{T_3}{2} \psi
\]

\[
\hat{P}^1 = Z_{S^0} \hat{\psi} \gamma_5 \hat{\psi} + a^{-3}i\rho_p (am_q, \epsilon_q) \mathbb{1}
\]

\[
\hat{P}^b = Z_P \hat{\psi} \gamma_5 \hat{\psi} , \quad b = 2, 3
\]

\[
\hat{P}^0 = Z_S \bar{\psi} \gamma_5 \psi
\]

\[
\hat{S}^1 = Z_{S^0} \frac{\hat{\psi}}{2} \psi
\]

\[
\hat{S}^2 = Z_S \frac{\bar{\psi}}{2} \psi
\]

\[
\hat{m}_q = Z_P^{-1} m_q \quad \hat{\epsilon}_q = Z_S^{-1} \epsilon_q .
\]

As expected, the above formulae turn into eqs. (33) to (36) if we set \( \epsilon_q = 0 \) and perform the cyclic permutation of flavour indices \( 3 \to 2 \to 1 \to 3 \).

The above WTI's allow us to identify

\[
\hat{m}_q^{(+)} = \hat{m}_q + \hat{\epsilon}_q = Z_P^{-1} m_q + Z_S^{-1} \epsilon_q ,
\]

\[
\hat{m}_q^{(-)} = \hat{m}_q - \hat{\epsilon}_q = Z_P^{-1} m_q - Z_S^{-1} \epsilon_q
\]

as the renormalized masses of the quarks in the doublet.

For completeness we record the formulae

\[
\hat{S}^0 = Z_P \left[ \hat{\psi} \hat{\psi} + a^{-2} m_q \rho_{S^0} (am_q, \epsilon_q) \mathbb{1} \right]
\]

\[
\hat{S}^3 = Z_S \left[ \frac{\hat{\psi} \gamma_5 \hat{\psi}}{2} + a^{-2} \epsilon_q \rho_S (am_q, \epsilon_q) \mathbb{1} \right],
\]

where \( \rho_{S^0} (am_q, \epsilon_q) \) and \( \rho_S (am_q, \epsilon_q) \), as well as \( \rho_P (am_q, \epsilon_q) \), are dimensionless real coefficients that admit a polynomial expansion both in \( am_q \) and \( \epsilon_q \). The mixing coefficients \( \rho_P (am_q, \epsilon_q) \) and \( \rho_{S^0} (am_q) \), appearing in eqs. (41) and (42) in the mass degenerate case, coincide with the value at \( \epsilon_q = 0 \) of the coefficients introduced in eq. (35) and (33), respectively.

3.2. O(\( a \)) improvement

The method for O(\( a \)) improvement is just as in the mass degenerate case. The physical explanation of this fact is obvious: all O(\( a \)) discretization effects come from the Wilson term which is of the same form in the actions (4) and (33) (up to a trivial flavour rotation). Formally, it is enough to observe that the action (35) is invariant under the transformations \( \mathcal{R}_5 \times D_4 \) and

\[
\mathcal{R}_5^{spND} \equiv \quad \mathbb{1} \quad \mathbb{1} \quad \mathbb{1} \quad \mathbb{1} \quad \mathbb{1}
\]

\[
\mathbb{1} \quad \mathbb{1} \quad \mathbb{1} \quad \mathbb{1} \quad \mathbb{1}
\]

as well as under the spurionic parity operation (26). Invariance under \( \mathcal{R}_5^{spND} \) and \( \mathcal{R}_5 \times D_4 \) allows to prove (by arguments analogous to those presented in ref. (11)) that W.A's of energies and matrix elements are free from O(\( a \)) cutoff effects.

In formulæ (dropping the label \( \omega = \pi/2 \))

\[
E_{h,n}(k; m_q, \epsilon_q) + E_{h,n}(k; -m_q, \epsilon_q) =
\]

\[
= 2E_{h,n}^{cont}(k; m_q, \epsilon_q) + O(a^2),
\]

\[
\left[ (h, \epsilon, k) | B | h', \epsilon', k' \right]_{\{(r, m_q, \epsilon_q) \}} \mathbb{1} \times (r \to \bar{r}) =
\]

\[
= 2\zeta_B^H (r; n, k) | B | h', \epsilon', k' \rangle_{\{(r, m_q, \epsilon_q) \}} \mathbb{1} + O(a^2).
\]

Using the symmetry of the action (33) under the transformation (26), one can then prove, along the lines of sect. (22), that averages of ener-
gies evaluated with opposite values of the three-momenta as well as the appropriate linear combinations of matrix elements of m.r. operators taken between pairs of states with opposite external three-momenta are not affected by $O(a)$ discretization errors. In formulae

$$E_{h,n}(k; r, m_q, \epsilon_q) + E_{h,n}(-k; r, m_q, \epsilon_q) =$$

$$= 2E^\text{cont}_{h,n}(k; m_q, \epsilon_q) + O(a^2), \quad (48)$$

$$\langle h, n, k|B|h', n', k'\rangle\big|_{(r, m_q, \epsilon_q)} +$$

$$+ \eta^B_{hnh'n'}\langle h, n, -k|B|h', n', -k'\rangle\big|_{(r, m_q, \epsilon_q)} =$$

$$= 2\epsilon^B_{r}(r)\langle h, n, k|B|h', n', k'\rangle\big|_{(m_q, \epsilon_q)} + O(a^2). \quad (49)$$

3.3. The fermion determinant

The fermion determinant associated with the action \([33]\) is real and strictly positive, provided

$$m_q^2 > \epsilon^2. \quad (50)$$

The proof, though elementary, requires some algebra and is presented in detail in Appendix B.

It is important to realize that \([40]\) is not a trivial condition, because in terms of the renormalized quark masses, \(\hat{m}_q(\pm)\), it implies the inequality

$$\frac{Z_P}{Z_S} > \frac{\hat{m}_q^{(+)} - \hat{m}_q^{(-)}}{\hat{m}_q^{(+)} + \hat{m}_q^{(-)}}. \quad (51)$$

The latter leads to a rather stringent constraint on the (finite) ratio \(Z_P/Z_S\), if \(\hat{m}_q^{(+)} > \hat{m}_q^{(-)}\). One gets, in fact

$$\frac{Z_P}{Z_S} > 1 - \frac{2}{\hat{m}_q^{(+)} + \hat{m}_q^{(-)}} \left[\frac{\hat{m}_q^{(-)}}{\hat{m}_q^{(+)}}\right]^2. \quad (52)$$

Since numerically one finds \([40][41]\) for the quenched ratio \(Z_P/Z_S\) a number somewhat smaller than 1, one might be worried that the inequality \([41]\) is not fulfilled. On this issue a leverage can be offered by the choice of the value of \(r\) which can be any real number satisfying \(0 < |r| \leq 1\). In perturbation theory one finds for the standard Wilson action to one-loop \([6]\) something like \(Z_P/Z_S = 1 - g_0^2 r^2 I(r) + \ldots\), where \(I(r) = I(-r) > 0\) for \(0 < |r| \leq 1\) and has a finite limit at \(r = 0\). This suggests that decreasing \(|r|\) may increase \(Z_P/Z_S\).

4. Conclusions

In this note we have shown that tm-LQCD at \(\omega = \pm\pi/2\) yields a particularly useful lattice regularization of the Wilson type for the gauge theory of mass non-degenerate fermion pairs. Following ref. \([1]\), we have proved that with this action essentially all physically relevant quantities can be evaluated with no \(O(a)\) cutoff effects, while at the same time having the fermion determinant real and strictly positive, provided \(0 < \epsilon^2_q < m^2_q\).

Monte Carlo simulations are hence safely feasible. The difficulties of the standard HMC in the presence of a flavour non-diagonal structure of the WD operator, \(D_{\text{ND}}\) (see eq. \([42]\)), can be overcome e.g. by stochastically computing its determinant using algorithms of the multi-boson \([12]\) or PHMC \([13]\) type. Such algorithms should now be based on some polynomial approximation of \(1/\sqrt{D^1_{\text{ND}}D_{\text{ND}}}\) and naturally allow a simple correction of the employed polynomial approximation.

The approach we have discussed can be adapted \([5]\) to the calculation of matrix elements of the CP-conserving, \(\Delta S = 2\) and \(\Delta S = 1\) effective weak Hamiltonian, in a way which we expect will solve the problem of “wrong chirality mixings” in the construction of the corresponding m.r. lattice operators.

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Appendix A: Symmetries of the action \([33]\) and absence of counter-terms

We want to show that the (spurionic) symmetries enjoyed by the fermionic action \([33]\) ensure
that no extra operators (of dimension ≤ 4) can be generated by radiative corrections, besides those already present. The discussion that follows applies in particular to the case ε_q = 0, implying the “stability” under radiative corrections of the action \( \Theta \). 5

The list of transformations which leave the action \( \Theta \) invariant include

1) lattice gauge transformations, space-time translations and hyper-cubic rotations, as well as the \( U_V(1) \) vector transformation associated to baryon number conservation (none of these will play any special role in the discussion)

2) three continuous (one vector, \( I^1(\theta_1) \), and two axial, \( I^2(\theta_2) \), \( I^3(\theta_3) \)) non-singlet spurionic transformations

\[
\begin{align*}
\mathcal{I}^1(\theta_1) & \times (m_q + \epsilon_q \tau_3) \rightarrow e^{i \theta_1 \tau_1 / 2} (m_q + \epsilon_q \tau_3) e^{-i \theta_1 \tau_1 / 2}, \\
\mathcal{I}^2(\theta_2) & \times (m_q + \epsilon_q \tau_3) \rightarrow e^{i \theta_2 \gamma_5 \tau_2 / 2} (m_q + \epsilon_q \tau_3) e^{i \theta_2 \gamma_5 \tau_2 / 2}, \\
\mathcal{I}^3(\theta_3) & \times (m_q + \epsilon_q \tau_3) \rightarrow e^{-i \theta_3 \gamma_5 \tau_2 / 2} (m_q + \epsilon_q \tau_3) e^{-i \theta_3 \gamma_5 \tau_2 / 2},
\end{align*}
\]

where (notice the simplification occurring if \( b = 1 \))

\[
\mathcal{I}^3(\theta) \equiv \left\{ \begin{array}{ll}
\psi(x) & \rightarrow e^{i \gamma_5 \tau_1 / 4} e^{i \theta_3 \gamma_5 / 2} e^{-i \gamma_5 \tau_1 / 4} \psi(x) \\
\bar{\psi}(\tau_3) & \rightarrow -i \bar{\psi}^T(\tau_3) \gamma_0 \gamma_2
\end{array} \right.
\]

3) charge conjugation, \( \mathcal{C} \)

\[
\mathcal{C} : \left\{ \begin{array}{ll}
U_\mu(x) & \rightarrow U_\mu^T(x) \\
\bar{\psi}(x) & \rightarrow i \gamma_0 \gamma_2 \bar{\psi}^T(x) \\
\bar{\psi}(\tau_3) & \rightarrow -i \bar{\psi}^T(\tau_3) \gamma_0 \gamma_2
\end{array} \right.
\]

4) the (anti-linear) reflection operation, \( \Theta \). It can be defined either with respect to the time slice \( x_0 = 0 \) (site reflection, \( \Theta_s \)) or \( x_0 = a / 2 \) (link reflection, \( \Theta_l \)). Its action on monomials of fermionic fields is

\[
\Theta[f(U)\psi(x_1) \ldots \bar{\psi}(x_n)] = f^*(\Theta[U])\Theta[\bar{\psi}(x_n)] \ldots \Theta[\psi(x_1)],
\]

where \( f(U) \) is a functional of link variables and

\[
\Theta_{s/l}[U_{k}(x)] = U_{k}(\theta_{s/l}x),
\]

where (notice the simplification occuring if \( \epsilon_q = 0 \)) by the harmless flavour rotation \( \psi \rightarrow \exp(-i \tau_2 \pi / 4) \psi, \bar{\psi} \rightarrow \bar{\psi} \exp(i \tau_2 \pi / 4) \).

5) the pseudo-parity transformations

\[
\mathcal{P}_{1/2}^1 : \left\{ \begin{array}{ll}
U_0(x) & \rightarrow U_0(x_P), \\
U_k(x) & \rightarrow U_k(x_P - a \hat{k}), \quad k = 1, 2, 3
\end{array} \right.
\]

\[
\mathcal{P}_{F}^{2,3} : \left\{ \begin{array}{ll}
\psi(x) & \rightarrow i \tau_3 \gamma_0 \psi(x_P), \\
\bar{\psi}(x) & \rightarrow -i \bar{\psi}(x_P) \gamma_0 \tau_2
\end{array} \right.
\]

6) the transformation \( \mathcal{R}_5 \times \mathcal{D}_d \), where

\[
\mathcal{R}_5 : \left\{ \begin{array}{ll}
\psi(x) & \rightarrow \gamma_5 \psi(x) \\
\bar{\psi}(x) & \rightarrow -\bar{\psi}(x) \gamma_5
\end{array} \right.
\]

\[
\mathcal{D}_d : \left\{ \begin{array}{ll}
U_\mu(x) & \rightarrow U_\mu(-x - a \hat{\mu}) \\
\psi(x) & \rightarrow e^{i \tau_3 \gamma_0 / 2} \psi(-x) \\
\bar{\psi}(x) & \rightarrow e^{i \tau_3 \gamma_0 / 2} \bar{\psi}(-x)
\end{array} \right.
\]

7) the spurionic transformations \( \mathcal{E} \) and \( \mathcal{T}_E \times (r \rightarrow -r) \), where \( \mathcal{T}_E \) is the (euclidean) time-axis inversion. The action of \( \mathcal{T}_E \) on the elementary fields of the theory is \( (x_T \equiv (x, -x_0)) \)

\[
\mathcal{T}_E : \left\{ \begin{array}{ll}
U_0(x) & \rightarrow U_0^T(x_T - a \hat{0}) \\
U_k(x) & \rightarrow U_k(x_T), \quad k = 1, 2, 3 \\
\psi(x) & \rightarrow \gamma_5 \gamma_0 \psi(x_T) \\
\bar{\psi}(x) & \rightarrow \bar{\psi}(x_T) \gamma_0 \gamma_5
\end{array} \right.
\]

In Tables 1 and 2 we list all the independent operators of dimension not larger than 4 that cannot appear in the action \( \Theta \). They are grouped in columns under the name of the corresponding “killing” symmetry. The reality properties of the various coefficients in the action \( \Theta \) are fixed by the invariance under the anti-linear reflection operation \( \Theta_l \) (or \( \Theta_s \)).
Table 1
We list under the name of the relevant symmetry that forbids them all the operators of dimension \( d = 4 \) and \( d = 3 \) that cannot appear in the density action \((33)\). By \( \mathcal{F} \) we mean any lattice discretization of \( \epsilon_{\mu \nu \lambda} \epsilon_{\rho \sigma} \text{Tr}[F_{\mu \nu} F_{\lambda \rho}] \).

| Dim | \( \mathcal{C} \)          |
|-----|---------------------------|
| \( d = 4 \) | \( \bar{\psi} T \gamma_5 \nabla \psi \) (\( T = 1, \tau_1, \tau_3 \)) |
| \( d = 3 \) | \( \bar{\psi} \tau_2 \psi \) |

Table 2
Continuation of Table 1

| Dim | \( P_F^2 \) | \( P_F^2 \times (\epsilon_q \rightarrow -\epsilon_q) \) |
|-----|-------------|----------------------------------|
| \( d = 4 \) | \( \bar{\psi} T \gamma_5 \nabla \psi \) (\( T = \tau_1, \tau_2 \)) | \( \bar{\psi} T \gamma_2 \gamma_5 \nabla \psi \) |
| \( d = 3 \) | \( \bar{\psi} \gamma_5 \psi \) | \( \bar{\psi} \gamma_3 \nabla \psi \) |

The conclusion of this discussion is that the form \((33)\) of the action is preserved by radiative corrections and the bare parameters, \( g_0^2 \), \( m_q \), and \( \epsilon_q \), need only a purely multiplicative renormalization. More details on the renormalization of \( m_q \) and \( \epsilon_q \) can be found in the text in sect. \ref{sect:renormalization}.

Appendix B: Positivity of the fermion determinant

In this Appendix we show that under the condition \((50)\) the determinant of the WD operator associated with the action \((33)\), namely

\[
D_{\text{ND}} = \gamma \cdot \nabla - i \gamma_5 \tau_1 W_{\text{cr}}(r) + m_q + \gamma_3 \epsilon_q , \quad (67)
\]

is real and (strictly) positive. To prove that \( D_{\text{F,ND}} = \text{Det}[D_{\text{ND}}] \) is a real number it is enough to note the self-adjointness relation

\[
\gamma_5 \tau_3 D_{\text{ND}} \gamma_5 \tau_3 = D_{\text{ND}}^\dagger . \quad (68)
\]

The proof of positivity is somewhat more involved. To proceed it is convenient to introduce the auxiliary self-adjoint operator

\[
Q_{\text{cr}} = \gamma_5 \left[ \gamma \cdot \nabla + W_{\text{cr}}(r) \right] = Q_{\text{cr}}^\dagger , \quad (69)
\]

in terms of which \( D_{\text{F,ND}} \) can be written in the form

\[
D_{\text{F,ND}} = \text{Det}[Q_{\text{cr}} + i \tau_1 m_q + \gamma_5 \tau_3 \epsilon_q] . \quad (70)
\]

In flavour space the operator in the r.h.s. of eq. \((70)\) is represented by the \( 2 \times 2 \) matrix

\[
Q_{\text{cr}} + i \tau_1 m_q + \gamma_5 \tau_3 \epsilon_q = \gamma_5 e^{i \gamma_5 \gamma_3/4} D_{\text{ND}} e^{i \gamma_5 \gamma_3/4}
\]

\[
= \begin{pmatrix} Q_{\text{cr}} + \gamma_5 \epsilon_q & im_q \\ im_q & Q_{\text{cr}} - \gamma_5 \epsilon_q \end{pmatrix} . \quad (71)
\]

For the determinant of this operator one finds

\[
D_{\text{F,ND}} = \text{Det}[D_{\text{ND}}] = \\
= \text{Det}[(Q_{\text{cr}} + \gamma_5 \epsilon_q)(Q_{\text{cr}} - \gamma_5 \epsilon_q) + m_q^2] = \\
= \text{Det}[Q_{\text{cr}}^2 + m_q^2 - \epsilon_q^2 + 2 \epsilon_q \gamma \cdot \nabla] = \\
= \text{Det}[Q_{\text{cr}}^2 + m_q^2 - \epsilon_q^2] \cdot \text{Det}[1 + 2 \epsilon_q B] , \quad (72)
\]

where we have introduced the definition

\[
B = X \gamma \cdot \nabla X , \quad X = (Q_{\text{cr}}^2 + m_q^2 - \epsilon_q^2)^{-1/2} . \quad (73)
\]

Since \( \text{Det}[Q_{\text{cr}}^2 + m_q^2 - \epsilon_q^2] > 0 \), we only have to prove that the second factor in the last equality of \((72)\) is a positive quantity. To this end we observe that both \( D_{\text{F,ND}} \) (from eq. \((70)\) and \( \text{Det}[Q_{\text{cr}}^2 + m_q^2 - \epsilon_q^2] \) (by inspection) are even under \( \epsilon_q \rightarrow -\epsilon_q \). We then conclude that

\[
\Delta_{\text{F,ND}}(\epsilon_q) \equiv \text{Det}[1 + 2 \epsilon_q B] = \Delta_{\text{F,ND}}(-\epsilon_q) . \quad (74)
\]

This property is indeed enough to prove the positivity of \( \Delta_{\text{F,ND}} \) and hence our thesis. Let us consider, in fact, the expansion

\[
\text{tr}[\log(1 + 2 \epsilon_q B)] = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} (2 \epsilon_q)^k \text{tr}[B^k] , \quad (75)
\]

valid for sufficiently small values of \( \epsilon_q \)\(^6\). Eq. \((74)\) implies that only even powers of \( \epsilon_q \) can contribute. This fact together with the observation

\(^6\) For instance, one can take \( 2|\epsilon_q| \) smaller than the number \( \min \{m_q, 1/|B|2\epsilon_q=m_q\} \).
that $B$ is an anti-Hermitian operator ($B^\dagger = -B$, because $\gamma \cdot \nabla$ is anti-Hermitian) allows us to write

$$\text{l.h.s. of (75)} = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{2n} (2\epsilon_q)^{2n} \text{tr}[(B^\dagger B)^n] = \frac{1}{2} \text{tr}[\log(1 + 4\epsilon_q^2 B^\dagger B)].$$

(76)

The last equality proves that $\text{tr}[\log(1 + 2\epsilon_q B)]$ is a non-negative quantity, implying that $\text{det}[1 + 2\epsilon_q B]$ is real and strictly positive.

We conclude with two technical observations: 1) since $B$ is anti-Hermitian, its spectrum is purely imaginary, thus $1 + 2\epsilon_q B$ cannot have any vanishing eigenvalue; 2) eq. (76), which was proved for sufficiently small $\epsilon_q$, can be extended to the actual physical value of the mass splitting by analyticity (see the chain of equalities in eq. (72)).

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