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Twisted mass lattice QCD

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Abstract

I review the theoretical foundations, properties as well as the simulation results obtained so far of a variant of the Wilson lattice QCD formulation: Wilson twisted mass lattice QCD. Emphasis is put on the discretization errors and on the effects of these discretization errors on the phase structure for Wilson-like fermions in the chiral limit. The possibility to use in lattice simulations different lattice actions for sea and valence quarks to ease the renormalization patterns of phenomenologically relevant local operators, is also discussed.

Key words: lattice QCD, O(a) improvement, chiral perturbation theory, renormalization

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1 Introduction

Quantum Chromodynamics (QCD) is today considered the fundamental theory of strong interactions. The adimensional coupling of the theory g_0, once it is renormalized, will depend on the energy scale of the considered physical process, and it gives a measure of the strength of the interaction at that energy scale. The outstanding property of QCD, *asymptotic freedom*, tells us that the coupling decreases with increasing energies. This allows the usage of perturbation theory to make phenomenological predictions for processes with large momentum transfered. However the increase of the coupling with decreasing energies does not allow to use perturbative methods to compute physical quantities in the low energy region such as the mass spectrum or hadronic matrix elements. A possible strategy in this case is to use a non-perturbative regularization of the theory, introducing a discretized space-time (lattice) [1, 2]. This strategy has two main advantages: first it provides an ultraviolet regularization and secondly it reduces the degrees of freedom of the theory to a numerable infinity. Considering the theory in a finite volume lattice, it is possible to perform numerical simulations of QCD through Monte Carlo methods. The continuum QCD action has to be discretized in a sensible way, and a simple and attractive lattice action is the one proposed by Wilson long time ago [1, 2].

The relation between the coupling constant g_0 and the lattice spacing a in physical units is given, in lattice QCD, by the renormalization group equations, and we are naturally interested in the continuum limit of the theory. The simulations of lattice QCD are always performed for values of g_0 corresponding, in the renormalized theory, to a finite and non zero value of a. This introduces in the results of the simulations, using the Wilson fermion action, errors of order a and numerically these $\mathrm{O}(a)$ errors could be of the order of $20-30\%$. The $\mathrm{O}(a)$ discretization errors could be eliminated, in principle, following the Symanzik's improvement program [3–5], where the $\mathrm{O}(a)$ cutoff effects in on-shell quantities are canceled by adding local $\mathrm{O}(a)$ counterterms to the lattice action and to the composite fields of interest [6–10]. A technical difficulty is that the improvement coefficients multiplying these counterterms are not known a priori, and they should be all computed using Monte Carlo simulations.

A new intriguing possibility is the so called automatic $\mathrm{O}(a)$ improvement [11], where none of the improvement coefficients are needed in order to have $\mathrm{O}(a^2)$ cutoff effects in physical observables. The basic idea is that the Wilson theory for fermions with a suitable infrared cutoff is in the massless limit free from $\mathrm{O}(a)$ errors. We will see that to extend automatic $\mathrm{O}(a)$ improvement to a theory in infinite volume with a non zero mass term we have to add the so called *twisted mass*, keeping the standard quark mass to be zero. The twisted mass term, that in a way will act also as a sharp infrared cutoff, can be obtained in continuum QCD via a non-anomalous chiral rotation from the standard mass term. To be specific, if we consider QCD with a

field χ describing a flavour doublet, the twisted mass term looks like

$$i\mu_{\rm q}\overline{\chi}\gamma_5\tau^3\chi \tag{1.1}$$

where τ^3 is the Pauli matrix in flavour space and $\mu_{\rm q}$ is what is called twisted mass.

The twisted mass term in a lattice QCD action appears to my knowledge for the first time in ref. [12], where it is given an ansatz for the phase structure of Wilson fermions in the parameter space $m_0 - g_0^2$, where m_0 is the bare quark mass. Based on the analysis of the lattice Gross-Neveu model, and on the strong coupling expansion of Wilson lattice QCD, the author suggested that there are regions in the parameter space of g_0^2 and m_0 where the true vacuum has a non zero expectation value of $i\overline{\chi}\gamma_5\chi$ signalling the spontaneous breaking of parity symmetry. It was then natural to propose, in order to pick up the real vacuum from numerical simulations, to add an external field $iH\overline{\psi}\gamma_5\psi$ to the original lagrangian and to perform the limit $H \to 0^+$. The H is what now we would call twisted mass. The twisted mass in this case is then just an external field used to probe the structure of the vacuum of the theory and it has to be removed at the end of the computation. We will come back in deatil to the chiral phase structure of the Wilson theory in sect.5. Here I just would like to mention that in the same paper a new method to improve the scaling behaviour of the chiral condensate was proposed based on the observation that the scaling violations of the condensate are odd under a change of sign of the coefficient of the Wilson term, and they can be easily averaged out. We will see in app. E that this is a possible starting point to understand automatic O(a) improvement.

The twisted mass term breaks parity and flavour symmetry. It is a natural question whether this mass term changes also the continuum action or just the discretization errors of the theory. In this report we will show that with a Wilson fermion lattice action the twisted mass term generates parity and flavour violating cutoff effects (in most cases of O(a^2)) which go away performing the continuum limit.

The fact that the twisted mass actually induces only flavour and parity breaking cutoff effects, and it is actually equivalent to QCD, can be understood considering an old remark made by Gasser and Leutwyler. In fact it was noticed many years ago [13] that the usage of what we would now call a twisted mass term is irrelevant in continuum QCD. The fermionic part of the 2 flavours QCD Lagrangian is usually given in the form

$$\mathcal{L}_{\rm QCD} = \overline{\chi}\Big[\gamma_\mu D_\mu + \mathbf{m}\Big]\chi \tag{1.2}$$

where $\mathbf{m}$ is the mass matrix. The quark masses in the standard model originate from the asymmetries of the electroweak vacuum. Since the electroweak interactions do not preserve parity there is no reason a priori for the quark mass term of QCD to be parity invariant, and can be generically written as $\overline{\chi}(\mathbf{m} + i\gamma_5\boldsymbol{\mu})\chi$. We assume here that $\boldsymbol{\mu}$ is a traceless matrix to avoid an unnecessary discussion of the QCD vacuum angle. With a suitable non-anomalous chiral transformation of the quark fields the

general mass term $\overline{\chi}(\mathbf{m}+i\gamma_5\boldsymbol{\mu})\chi$ can always be brought to the standard form, where the mass matrix is diagonal with real positive eigenvalues $m_{\rm u}$ and $m_{\rm d}$. The remaining part of the Lagrangian constrained by the requirement of renormalizability is left invariant by this chiral transformation. In brief, with a change of variables in the functional integral, that leaves the measure invariant, one can show that even if a general parity and flavour violating mass term is allowed, the request of having a renormalizable theory preserving gauge and Lorentz invariance, generates these "accidental symmetries". This simple example shows that the specific form of the mass term in the 2 flavours continuum QCD Lagrangian is actually irrelevant. The reason for this is the fact that the massless theory is invariant under the chiral non-anomalous transformation that changes the form of the mass term.

This is just an example of a more general phenomenon. Renormalizable theories that describe electro-weak and strong interactions, can be considered as low energy effective theories of more general not necessarily renormalizable high energy theories. The condition of having low energy renormalizable field theories can be so stringent that the corresponding Lagrangian may turn out to obey extra accidental symmetries, that were not symmetries of the higher energy theories [14].

This observation becomes important on the lattice. If we discretize the continuum QCD action with Wilson fermions [1], the Wilson term explicitly breaks chiral symmetry and the lattice action is not invariant anymore under the field rotations mentioned before. But we still have the freedom to choose the Wilson term and the mass term to point in different relative "directions" in the Dirac and flavour space [15]. This freedom is the key to constrain the form of the cutoff effects induced by the Wilson term.

The observation that physical observables computed with the Wilson lattice action are automatically O(a) improved in the "infrared safe" (i.e. with no spontaneous symmetry breaking) chiral limit is relevant also for the renormalization properties of local operators that depend on the breaking of chiral symmetry induced by the Wilson term.

To summarize: Wilson twisted mass QCD is a lattice regularization that allows automatic O(a) improvement only tuning one parameter. The bare untwisted quark mass m_0 has to be tuned to the so called critical mass in order to maximally disalign the Wilson term and the mass term. In this approach the renormalization of local operators relevant for phenomenological applications is significantly simplified with respect to the standard Wilson regularization. The price to pay is the existence of O(a^2) cutoff effects that break parity and flavour symmetry. All these statements will be demonstrated explicitly in this report.

This is not the only review on twisted mass QCD. A set of lectures has been presented by S.Sint at the School "Perspectives in Lattice Gauge Theories" [16]. In

these lectures a nice introduction on the basic setup, exceptional configurations, automatic O(a) improvement together with few applications of Wtm is given. Particular emphasis is also put in finite volume renormalization schemes with chirally twisted bounday conditions. In our report we enlarge the topics covered by Sint, and we elaborate on the ones already there. On the other side we touch only marginally finite volume renormalization schemes with chirally twisted bounday conditions. For this reason we believe that the present review is in many respects complementary to the one of Sint, and together they can be used as a complete introduction to all the topics connected with twisted mass QCD.

The paper is organized as follows. In section 2 I use classical considerations in continuum QCD to show the equivalence of twisted mass (tm) QCD and QCD. I also describe the rigorous theoretical properties of Wilson twisted mass QCD (Wtm QCD), for degenerate and non-degenerate quarks. In section 3 I discuss the O(a) discretization errors of Wilson-like lattice actions. In particular I show several proof of automatic O(a) improvement, with a particular emphasis on the choice of the critical mass. Numerical results confirming this property will conclude the section. In section 4 I derive again some of the results obtained in the previous sections using a different fermion basis. Hopefully this could help the reader in a better understanding of the subject of this review. In section 5 I analyse O(a^2) parity and isospin violating discretization errors and O(a^2) cutoff effects responsible for the non trivial chiral phase structure of the lattice theory. In section 6 I discuss selected numerical results obtained with Wtm QCD and show different methods to ease the renormalization of local operators. In section 7 I make a short digression on algorithms to simulate light Wilson-like quarks. This is an important prerequisite for part of the numerical results presented in this review. Conventions, notations and more technical discussions are deferred to the Appendix.

2 Basic properties

In this section we introduce twisted mass QCD in the continuum using classical arguments for a doublet of degenerate quarks. This academic exercise allows the reader to get acquainted with twisted mass QCD and to learn how to relate correlation functions from QCD to twisted mass QCD. To extend this concepts at a quantum level we discretize the theory on a lattice using Wilson fermions. The resulting theory Wilson twisted mass (Wtm) QCD is ultra-local, unitary, reflection positive and renormalizable to all orders in perturbation theory.

2.1 Twisted mass QCD in the continuum

We first consider the continuum limit of the twisted mass (tm) QCD action for $N_{\mathrm{f}} = 2$ degenerate quarks. We will always work in euclidean space and all the definitions and conventions are collected in app. A. We call the set of fermion fields $\{\chi, \overline{\chi}\}$ the *twisted* basis. In this basis the tm QCD action reads

$$S_{\mathrm{F}}[\chi, \overline{\chi}, G] = \int \mathrm{d}^4x\, \overline{\chi} \left(\gamma_\mu D_\mu + m_{\mathrm{q}} + i\mu_{\mathrm{q}}\gamma_5\tau^3\right) \chi, \tag{2.1}$$

where $D_\mu = \partial_\mu + G_\mu$ denotes the covariant derivative in a given gauge field G_μ, and τ^3 is the third Pauli matrix acting in flavour space. To better understand the structure of the action we write explicitly all the indices. The fermion fields are

$$\chi_{A,\alpha,i}(x) \tag{2.2}$$

where A is the colour index, α the Dirac index and i the flavour index. The action then reads

$$\begin{aligned} S_{\mathrm{F}}[\chi, \overline{\chi}, G] = \int \mathrm{d}^4x\, \overline{\chi}_{A,\alpha,i}(x)\, \big((\gamma_\mu)_{\alpha\beta}(D_\mu)_{AB}\delta_{ij} + (m_{\mathrm{q}})\delta_{AB}\delta_{\alpha\beta}\delta_{ij} \\ + (i\mu_{\mathrm{q}})(\gamma_5)_{\alpha\beta}(\tau^3)_{ij}\delta_{AB}\big)\, \chi_{B,\beta,j}(x). \end{aligned} \tag{2.3}$$

In the following we will use the compact notation in order to keep the reading not too heavy. The mass term of the tm action can be written as

$$m_{\mathrm{q}} + i\mu_{\mathrm{q}}\gamma_5\tau^3 = M\mathrm{e}^{i\alpha\gamma_5\tau^3} \tag{2.4}$$

where

$$M = \sqrt{m_{\mathrm{q}}^2 + \mu_{\mathrm{q}}^2} \tag{2.5}$$

is the so called polar mass. At the moment the tmQCD action is just a rewriting of standard QCD in a different basis. In fact performing the following axial transfor-

mation

$$\psi = \exp(i\omega\gamma_5\tau^3/2)\chi, \qquad \overline{\psi} = \overline{\chi}\exp(i\omega\gamma_5\tau^3/2), \tag{2.6}$$

the form of the action is left invariant, but the mass term transforms into

$$M\mathrm{e}^{i(\alpha-\omega)\gamma_5\tau^3}. \tag{2.7}$$

In particular, the standard QCD action for $N_\mathrm{f} = 2$ degenerate quarks

$$S_\mathrm{F}[\psi, \overline{\psi}, G] = \int \mathrm{d}^4x\, \overline{\psi}\,(\gamma_\mu D_\mu + M)\,\psi, \tag{2.8}$$

is obtained if $\omega = \alpha$, i.e. if the *twist angle* ω satisfies the relation

$$\tan\omega = \mu_\mathrm{q}/m_\mathrm{q}. \tag{2.9}$$

We call the *physical basis* $\{\psi, \overline{\psi}\}$ the basis where the continuum QCD action takes the standard form. The two basis are related by the rotation (2.6) with ω satisfying eq. (2.9).

In the following we will mainly use the *twisted* basis since this is the basis used in the numerical simulations. Although the physical interpretation of the fermionic correlation functions is most transparent in the *physical* basis the renormalization of gauge–invariant correlation functions, including those with insertions of local operators, looks simpler in the *twisted* basis. This will become clear later when we will discretize the action (2.1) using Wilson fermions [1, 2]. In sect. 5 I derive again some results in the physical basis.

Twisted mass QCD (2.1) and standard QCD (2.8) actions are exactly related by the transformation (2.6) and therefore share all the symmetries. The symmetry transformations in the *twisted* basis are simply the transcription of the standard symmetry transformations using eq. (2.6). These symmetry transformations will be from now on called *twisted* symmetries and they are collected in app. B. The twisted vector symmetry $SU_\mathrm{V}(2)_\omega$ defined in eq. (B.1) is a symmetry of the tmQCD action (2.1), while the mass term M breaks the twisted axial symmetry $SU_\mathrm{A}(2)_\omega$ defined in eq. (B.2). This is equivalent to the transformation properties of the QCD action (2.8) under the standard $SU_\mathrm{V}(2)$ and $SU_\mathrm{A}(2)$ symmetries transformations.

In order to give the correct physical interpretation of the interpolating fields in the twisted basis it is important to have available the relations between the currents in the two basis. The axial and vector currents are

$$A^a_\mu = \overline{\chi}\gamma_\mu\gamma_5\frac{\tau^a}{2}\chi, \qquad V^a_\mu = \overline{\chi}\gamma_\mu\frac{\tau^a}{2}\chi, \tag{2.10}$$

while the pseudoscalar and scalar densities are defined by

$$P^a = \overline{\chi}\gamma_5\frac{\tau^a}{2}\chi, \qquad S^0 = \overline{\chi}\chi. \tag{2.11}$$

The axial transformation (2.6) of the quark and anti-quark fields induces a transformation of the composite fields. We indicate with a calligraphic symbol the corresponding currents in the physical basis. For example, the rotated axial and vector currents read,

$$\mathcal{A}^a_\mu \equiv \overline{\psi}\gamma_\mu\gamma_5\frac{\tau^a}{2}\psi = \begin{cases}\cos(\omega)A^a_\mu + \varepsilon^{3ab}\sin(\omega)V^b_\mu & (a=1,2),\\ A^3_\mu & (a=3),\end{cases} \tag{2.12}$$

$$\mathcal{V}^a_\mu \equiv \overline{\psi}\gamma_\mu\frac{\tau^a}{2}\psi \;\; = \begin{cases}\cos(\omega)V^a_\mu + \varepsilon^{3ab}\sin(\omega)A^b_\mu & (a=1,2),\\ V^3_\mu & (a=3),\end{cases} \tag{2.13}$$

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

$$\mathcal{P}^a \equiv \overline{\psi}\gamma_5\frac{\tau^a}{2}\psi = \begin{cases}P^a & (a=1,2),\\ \cos(\omega)P^3 + i\sin(\omega)\frac{1}{2}S^0 & (a=3),\end{cases} \tag{2.14}$$

$$\mathcal{S}^0 \equiv \overline{\psi}\psi = \cos(\omega)S^0 + 2i\sin(\omega)P^3. \tag{2.15}$$

The same procedure to change basis can be used for any local operator. In app. F we give the example for a proton interpolating field.

The form of the Ward identities in the *twisted basis* is slightly different from the standard form. The local $SU_{\rm V}(2)\times SU_{\rm A}(2)$ chiral transformations of the fermionic fields are defined as follows

$$\delta\chi(x) = i\Big[\alpha^a_V(x)\frac{\tau^a}{2} + \alpha^a_A(x)\frac{\tau^a}{2}\gamma_5\Big]\chi(x) \tag{2.16}$$

$$\delta\overline{\chi}(x) = i\overline{\chi}(x)\Big[-\alpha^a_V(x)\frac{\tau^a}{2} + \alpha^a_A(x)\frac{\tau^a}{2}\gamma_5\Big], \tag{2.17}$$

and the symmetry at the classical level ($\delta S = 0$ where δ indicates the variations on the fermion fields of eqs. 2.16 - 2.17) gives the so-called partially conserved axial current (PCAC) and partially conserved vector current (PCVC) relations

$$\partial_\mu A^a_\mu = 2m_{\rm q}P^a + i\mu_{\rm q}\delta^{3a}S^0, \tag{2.18}$$

$$\partial_\mu V^a_\mu = -2\mu_{\rm q}\,\varepsilon^{3ab}P^b. \tag{2.19}$$

It is easy to verify that the rotated currents and densities satisfy the Ward identities in their standard form,

$$\partial_\mu\mathcal{A}^a_\mu = 2M\mathcal{P}^a, \qquad \partial_\mu\mathcal{V}^a_\mu = 0, \tag{2.20}$$

if ω is related to the mass parameters as in eq. (2.9). The PCAC and PCVC masses that appear in eqs. (2.18,2.19) are the 2 components of the physical mass which is given by the polar mass M (see eqs. 2.5 and 2.20). A particular case is when one of

the 2 masses vanishes: then the physical mass is given by the non-vanishing mass. We will see in the following that a very interesting case is when we work at *full twist*, also called *maximal twist*. Full twist corresponds at the classical level to $m_{\rm q} = 0$ or equivalently to $\omega = \pi/2$. In this case the role of the physical mass is fully played by the twisted mass $\mu_{\rm q}$.

2.2 Beyond the classical theory

These classical considerations, based on the possibility of performing the axial transformation (2.6) on the fermion fields, show that there is a one-to-one correspondence between tmQCD and standard QCD.

Denoting the sum of the gauge and fermion QCD actions by $S = S_G + S_F$, the physical content of the quantum theory can be extracted from its n-point correlation functions

$$\langle \mathcal{O}(x_1, \ldots, x_n) \rangle = \mathcal{Z}^{-1} \int D[\psi, \overline{\psi}] D[U] \, \mathrm{e}^{-S} \mathcal{O}(x_1, \ldots, x_n), \tag{2.21}$$

with

$$\mathcal{Z} = \int D[\overline{\chi}, \chi] D[U] \, \mathrm{e}^{-S}, \tag{2.22}$$

where $\mathcal{O}(x_1, \ldots, x_n)$ is a product of local gauge invariant composite fields which are localised at the space time points $x_1, \ldots, x_n$. For the discussion of this subsection we concentrate on the dependence of the correlation functions on the fermionic fields and on the mass. Formally in the functional integral (2.21) we can make the axial change of variables (2.6). This change of variables is non anomalous, i.e. it does not change the integration measure. As we have already discussed in the previous subsection only the mass term of the action is affected. Then the relation between correlation functions in the two basis reads

$$\langle \mathcal{O}[\psi, \overline{\psi}] \rangle_{(M,0)} = \langle O[\chi, \overline{\chi}] \rangle_{(m_{\rm q}, \mu_{\rm q})} \tag{2.23}$$

where the index of the correlation function in the l.h.s indicates that it has been computed in standard QCD with quark mass M and the index of the correlation function in the r.h.s indicates that it has been computed in tmQCD with quark masses $m_{\rm q}$ and $\mu_{\rm q}$. The relation between the arguments of the correlation function is given exactly by eq. (2.6). An explicit example of eq. (2.23) reads

$$\langle \mathcal{A}^1_\mu(x) \mathcal{P}^1(y) \rangle_{(M,0)} = \cos\omega \langle A^1_\mu(x) P^1(y) \rangle_{(m_{\rm q}, \mu_{\rm q})} + \sin\omega \langle V^2_\mu(x) P^1(y) \rangle_{(m_{\rm q}, \mu_{\rm q})}. \tag{2.24}$$

Correlation functions in QCD can be written as a linear combination of correlation functions computed in tmQCD at a given twist ω.

This equivalence remains valid at finite lattice spacing for Wilson fermions up to discretization errors, if the theory is correctly renormalized in a mass independent scheme [15].

To carry over these formal considerations to a rigorous level, we have to regularize the theory with a regulator which preserves the chiral symmetry of the massless theory, i.e. which preserves the axial symmetry containing the transformation (2.6). A chiral invariant regularization is provided by Ginsparg-Wilson (GW) quarks [17] on the lattice.

With GW fermions we can repeat the same steps performed formally in the continuum theory. In particular with GW fermions eq. (2.23) is valid in the bare theory, and analogously the bare Ward identity masses coincide with the bare mass parameters of the action. Using then Ginsparg-Wilson fermions as a theoretical tool it is possible to prove [15] that tmQCD and QCD are equivalent, i.e. given a lattice regularization that preserves chiral symmetry, the one-to-one correspondence between tmQCD and standard QCD is preserved at *finite lattice spacing*: consequently they have the same continuum limit. There is only one condition that has to be fulfilled for this statement to be true: all multiplicative renormalization constants have to be independent of the angle ω, not only up to cutoff effects [15]. A simple example of a suitable renormalization scheme of this kind is a mass-independent scheme which is obtained by renormalizing the theory in the chiral limit. Under this condition then the relations between renormalized correlation functions take the analogous form given by classical considerations. In other words in the continuum or with GW fermions, there is no reason to introduce a twisted mass term: it can be rotated away by a change of variable in the functional integral, because in both cases the massless theories are chirally symmetric.

Based on universality one then expects that tmQCD in other, not necessarily chirally invariant, regularizations can again be renormalized such that equivalence between renormalized correlation functions computed in tmQCD and standard QCD is satisfied up to cutoff effects [15]. In particular if the regulated theory breaks chiral symmetry even in the massless limit the twisted mass term cannot be rotated away and the twist angle ω parametrizes a family of regularizations, which differ at finite lattice spacing, but have the same continuum limit. It may hence be advantageous to choose the twist angle in a suitable way, e.g. to reduce discretization errors.

The relations between local fields in the classical continuum theory, e.g. eqs. (2.12,2.13), thanks to the equivalence between tmQCD and QCD at the quantum level, can be extended to the renormalized theory. Thus the classical theory may be used as a guide to establish the relations between renormalized correlation functions. This is a very important result and we will come back on it in sect. 2.8, in order to better understand which are the relations between tmQCD and QCD correlation functions.

2.3 Wilson twisted mass QCD

We are interested to exploit the freedom given to us by the choice of the twist angle in order to improve the properties of chirally non-invariant Wilson regularization of lattice QCD.

The setup is a hypercubic infinite lattice, with lattice spacing a. Standard reference books for lattice field theories are [18–22]. The gauge group is $SU(N_{\rm c})$ and the gauge field on the lattice is an $SU(N_{\rm c})$ matrix $U(x;\mu)$ that depends on the lattice point and on the four directions. Fermion fields reside on the lattice sites and as we have explained in the previous section, they carry colour, Dirac and flavour indices. The lattice action for $N_{\rm f} = 2$ degenerate flavours is of the form

$$S[\chi,\overline{\chi},U] = S_G[U] + S_F[\chi,\overline{\chi},U], \tag{2.25}$$

where S_G denotes the Wilson plaquette action

$$S_G[U] = \frac{\beta}{6}\sum_{x;\mu\neq\nu}\mathrm{tr}\Big\{1 - P^{1\times 1}(x;\mu,\nu)\Big\}, \tag{2.26}$$

with $\beta = 6/g_0^2$, g_0 being the bare gauge coupling and $P^{1\times 1}(x;\mu,\nu)$ the parallel transporter around a plaquette P

$$P^{1\times 1}(x;\mu,\nu) = U(x;\mu)U(x+a\hat{\mu};\nu)U(x+a\hat{\nu};\mu)^{-1}U(x;\nu)^{-1}. \tag{2.27}$$

The sum runs over all the oriented plaquettes P on the lattice. With Wilson quarks the tmQCD Dirac operator is given by

$$S_{\rm F}[\chi,\overline{\chi},U] = a^4\sum_x \overline{\chi}(x)\Big[D_{\rm W} + m_0 + i\mu_{\rm q}\gamma_5\tau^3\Big]\chi(x), \tag{2.28}$$

where

$$D_{\rm W} = \frac{1}{2}\{\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - ar\nabla^*_\mu\nabla_\mu\}, \tag{2.29}$$

∇_μ, ∇^*_μ are the standard gauge covariant forward and backward derivatives defined in app. A, m_0 and $\mu_{\rm q}$ are respectively the bare untwisted and twisted quark masses. The parameter r is the so called Wilson parameter and it is always set to 1 unless specified. We will call the action (2.28) the Wilson twisted mass (Wtm) QCD action. Sometimes Wilson actions are also written as

$$S_{\rm F}[\chi,\overline{\chi},U] = \sum_x \Big\{ \overline{\chi}(x) \Big[1 + i2\kappa a\mu_{\rm q}\gamma_5\tau^3 \Big] \chi(x) \\ - \kappa \sum_{\mu=0}^{3} \overline{\chi}(x) \Big[U(x;\mu)(1-\gamma_\mu)\chi(x+\hat{\mu}) \\ + U(x-\hat{\mu};\mu)^{-1}(1+\gamma_\mu)\chi(x-\hat{\mu}) \Big] \Big\}, \tag{2.30}$$

where we define the rescaled dimensionless fermion field

$$\chi \to \frac{\sqrt{2\kappa}}{a^{3/2}}\chi, \qquad x_\mu \to a x_\mu \tag{2.31}$$

and the hopping parameter

$$\kappa = \frac{1}{8+2am_0}. \tag{2.32}$$

The hopping parameter is an alternative way to label the bare untwisted quark mass, as β defined before is an alternative way to label the bare gauge coupling.

The first term of eq. (2.29) is a standard symmetric discretization of a lattice derivative and the second term

$$a\overline{\chi}\nabla^*_\mu\nabla_\mu\chi \tag{2.33}$$

is the so-called Wilson term. It can be easily checked that this term is not invariant under all the axial transformations, but it is needed in order to remove from the spectrum of the theory other spurious particles, called doublers, introduced by the lattice discretization. In the case of naive fermions, without the Wilson term, the existence of the doublers is related to the so called spectrum doubling symmetry [23], that can be seen as an exchange symmetry among the corners of the Brillouin zone in the reciprocal momentum space. It can be shown that the doubling phenomenon is a more general feature of ultra-local [1] actions that goes under the name of Nielsen-Ninomiya theorem [24, 25]. We will not go further into this topic, but since we are here interested in an action with a next-neighbour interaction (i.e. ultra-local) we need to insert a Wilson term.

The Wilson term (2.33) breaks explicitly the axial symmetry (2.6). This implies that the twisted mass term cannot be rotated away by a chiral transformation and the exact equivalence between the Wilson action with vanishing and non-vanishing twisted mass is lost: Wilson and Wilson twisted mass are different lattice regularization. As we have discussed in sect. 2.2 the exact equivalence is recovered only in the continuum limit.

[1] With ultra-local actions we think of actions where the interaction range is spread over a finite number of points of the lattice.

The introduction of a twisted mass and Wilson terms requires an analysis of symmetries. In sect. 2.1 we have already seen that at the classical level the symmetries of tmQCD are the transcriptions of the standard QCD symmetry transformations via the axial transformation (2.6). They are collected in app. B. In the regulated theory, the action given in (2.28) breaks some of the symmetries of the classical action (2.1). The Wilson term (2.33) breaks twisted parity $\mathcal{P}_\omega$ (B.3), twisted time reversal $\mathcal{T}_\omega$ (B.4), and twisted vector symmetry $SU_{\mathrm{V}}(2)_\omega$ (B.1). Wtm shares with standard Wilson fermions the following symmetries: gauge invariance, lattice rotations, translations and charge conjugation $\mathcal{C}$ (see app. B for the definition). The ordinary parity symmetry transformation

$$\mathcal{P}: \begin{cases} U(x_0,\mathbf{x};0) \to U(x_0,-\mathbf{x};0), \quad U(x_0,\mathbf{x};k) \to U^{-1}(x_0,-\mathbf{x}-a\hat{k};k), \quad k=1,\,2,\,3 \\ \chi(x_0,\mathbf{x}) \to \gamma_0\chi(x_0,-\mathbf{x}) \\ \overline{\chi}(x_0,\mathbf{x}) \to \overline{\chi}(x_0,-\mathbf{x})\gamma_0 \end{cases} \tag{2.34}$$

is only a symmetry if combined either with a discrete flavour rotation

$$\mathcal{P}_F^{1,2}: \begin{cases} U(x_0,\mathbf{x};0) \to U(x_0,-\mathbf{x};0), \quad U(x_0,\mathbf{x};k) \to U^{-1}(x_0,-\mathbf{x}-a\hat{k};k), \quad k=1,\,2,\,3 \\ \chi(x_0,\mathbf{x}) \to i\gamma_0\tau_{1,2}\chi_l(x_0,-\mathbf{x}) \\ \overline{\chi}(x_0,\mathbf{x}) \to -i\overline{\chi}(x_0,-\mathbf{x})\tau_{1,2}\gamma_0 \end{cases} \tag{2.35}$$

or with a sign change of the twisted mass term

$$\widetilde{\mathcal{P}} \equiv \mathcal{P} \times [\mu_{\mathrm{q}} \to -\mu_{\mathrm{q}}]\,. \tag{2.36}$$

The same holds for ordinary time-reversal

$$\mathcal{T}: \begin{cases} U(x_0,\mathbf{x};0) \to U^{-1}(-x_0-a,\mathbf{x};0), \quad U(x_0,\mathbf{x};k) \to U(-x_0,\mathbf{x};k), \quad k=1,\,2,\,3 \\ \chi(x_0,\mathbf{x}) \to i\gamma_0\gamma_5\chi(-x_0,\mathbf{x}) \\ \overline{\chi}(x_0,\mathbf{x}) \to -\overline{\chi}(-x_0,\mathbf{x})i\gamma_5\gamma_0 \end{cases} \tag{2.37}$$

which is only a symmetry if combined either with a discrete flavour rotation

$$\mathcal{T}_F^{1,2}: \begin{cases} U(x_0,\mathbf{x};0) \to U^{-1}(-x_0-a,\mathbf{x};0), \quad U(x_0,\mathbf{x};k) \to U(-x_0,\mathbf{x};k), \quad k=1,\,2,\,3 \\ \chi(x_0,\mathbf{x}) \to i\gamma_0\gamma_5\tau_{1,2}\chi_l(-x_0,\mathbf{x}) \\ \overline{\chi}(x_0,\mathbf{x}) \to -i\overline{\chi}(-x_0,\mathbf{x})\tau_{1,2}\gamma_5\gamma_0 \end{cases} \tag{2.38}$$

or with a sign change of the twisted mass term

$$\widetilde{\mathcal{T}} \equiv \mathcal{T} \times [\mu_{\mathrm{q}} \to -\mu_{\mathrm{q}}]\,. \tag{2.39}$$

Incidentally this implies that $\mathcal{CPT}$ is a symmetry of the lattice action (2.28). Concerning the continuous symmetries the ordinary isovector $SU_{\rm V}(2)$ symmetry is broken explicitly by the $\mu_{\rm q}$ term down to the $U_{\rm v}(1)_3$ subgroup with diagonal generator τ_3

$$U_{\rm V}(1)_3 : \begin{cases} \chi(x) \to \exp(i\frac{\alpha_V}{2}\tau^3)\chi(x), \\ \overline{\chi}(x) \to \overline{\chi}(x)\exp(-i\frac{\alpha_V}{2}\tau^3). \end{cases} \tag{2.40}$$

which is a symmetry of the lattice action (2.28) together with the $U(1)$ transformations associated with fermion number conservation.

2.4.1 Chiral symmetry at $\omega = \frac{\pi}{2}$

In this section we analyze the case of full twist, i.e. $\omega = \pi/2$, because for axial and vector transformations this is a special case. We will discuss in sect. 2.8 and extensively in sect. 4.3 how to tune, in a non-perturbative way, the twist angle ω, i.e. the bare untwisted quark mass m_0. For what follows it is enough to assume that m_0, i.e. ω, has been tuned appropriately.

The twisted "charged" axial transformations for $a = 1, 2$ and $\omega = \pi/2$ read

$$\left[U_{\rm A}(1)_{\frac{\pi}{2}}\right]_{1,2} : \begin{cases} \chi(x) \longrightarrow \frac{1}{\sqrt{2}}\left(1 - i\gamma_5\tau^3\right)\exp\left(i\frac{\alpha_A^{1,2}}{2}\gamma_5\tau^{1,2}\right)\frac{1}{\sqrt{2}}\left(1 + i\gamma_5\tau^3\right)\chi(x), \\ \overline{\chi}(x) \longrightarrow \overline{\chi}(x)\frac{1}{\sqrt{2}}\left(1 + i\gamma_5\tau^3\right)\exp(i\frac{\alpha_A^{1,2}}{2}\gamma_5\tau^{1,2})\frac{1}{\sqrt{2}}\left(1 - i\gamma_5\tau^3\right), \end{cases}$$

hence

$$\left[U_{\rm A}(1)_{\frac{\pi}{2}}\right]_{1,2} : \begin{cases} \chi(x) \longrightarrow \exp\left(\pm i\frac{\alpha_A^{1,2}}{2}\tau^{2,1}\right)\chi(x), \\ \overline{\chi}(x) \longrightarrow \overline{\chi}(x)\exp(\mp i\frac{\alpha_A^{1,2}}{2}\tau^{2,1}). \end{cases} \tag{2.41}$$

The twisted "charged" vector transformations for $a = 1, 2$ read

$$\left[U_{\rm V}(1)_{\frac{\pi}{2}}\right]_{1,2} : \begin{cases} \chi(x) \longrightarrow \exp\left(\pm i\frac{\alpha_V^{1,2}}{2}\gamma_5\tau^{2,1}\right)\chi(x), \\ \overline{\chi}(x) \longrightarrow \overline{\chi}(x)\exp(\pm i\frac{\alpha_V^{1,2}}{2}\gamma_5\tau^{2,1}). \end{cases} \tag{2.42}$$

For $\omega = \frac{\pi}{2}$ and for $a = 1, 2$ the form of the vector and axial transformations is reversed compared with the ordinary transformations. In the continuum this is really just a different transcription of the chiral transformations, coming from a different choice of the fermionic basis. On the contrary in the regulated theory different terms of the action break different sectors of the axial and vector transformations. In particular we observe that the Wilson term (2.33) breaks the "charged" twisted vector symmetry (2.42) and it is invariant under the "charged" twisted axial symmetry transformation (2.41). The twisted mass term has effectively an orthogonal behaviour because it is invariant under the "charged" twisted vector symmetry transformation (2.42) and it breaks the "charged" twisted axial symmetry (2.41).

To be more specific if we set the twisted mass to zero the Wilson theory is invariant under the group

$$\widetilde{SU}_{\rm A}(2) \equiv \left[U_{\rm A}(1)_{\frac{\pi}{2}}\right]_1 \otimes \left[U_{\rm A}(1)_{\frac{\pi}{2}}\right]_2 \otimes \left[U_{\rm V}(1)_{\frac{\pi}{2}}\right]_3 , \tag{2.43}$$

while the twisted mass term is invariant under the group

$$\widetilde{SU}_{\rm V}(2) \equiv \left[U_{\rm V}(1)_{\frac{\pi}{2}}\right]_1 \otimes \left[U_{\rm V}(1)_{\frac{\pi}{2}}\right]_2 \otimes \left[U_{\rm V}(1)_{\frac{\pi}{2}}\right]_3 . \tag{2.44}$$

This means that for the "charged" axial transformations the lattice action (2.28) [2] has a continuum-like behaviour: the twisted "charged" axial symmetry $\left[U_{\rm A}(1)_{\frac{\pi}{2}}\right]_{1,2}$ is only softly broken by the mass term. This exact symmetry of the massless theory protects the charged pion from chiral breaking cutoff effects (see eq. 4.74). This result is obviously independent on the choice of the basis and we will discuss it again in sect. 5. A consequence of this consideration is also that the charged vector current in the twisted basis is protected from renormalization and it is at the same time the current that defines the pseudoscalar decay constant for the charged pion (see eqs. 2.61,7.9,7.10). The neat result being that at full twist the pseudoscalar decay constant for the charged pion does not need to be renormalized (see sect. 7).

This analysis also shows in which sense the Wilson and the mass term at full twist are maximally disaligned: they are maximally disaligned concerning chiral symmetry. While the Wilson term breaks twisted "charged" flavour symmetry (2.42) the mass term breaks as in continuum QCD the full axial group (B.2), or to phrase it differently the Wilson term preserves a subgroup of twisted axial symmetry (2.41) while the mass term does not. What is relevant is that the Wilson and the mass term are "orthogonal" concerning the "charged" subgroup of chiral symmetry and this is achieved at full twist $\omega = \pi/2$.

2.5 Tree-level

To get some more insights on Wtm and to understand better the importance of disaligning mass term and Wilson term we compute here the tree-level Wtm propagator, that can be written as an integral over the first Brillouin zone of

$$\widetilde{G}(p) = \frac{-i\gamma_\mu \mathring{p}_\mu + \mathcal{M}(p) - i\mu_{\rm q}\gamma_5\tau^3}{\mathring{p}_\mu^2 + \mathcal{M}(p)^2 + \mu_{\rm q}^2} \tag{2.45}$$

where we have defined

$$\mathring{p}_\mu = \frac{1}{a}\sin(ap_\mu), \qquad \mathcal{M}(p) = m_0 + \frac{r}{2}a\hat{p}_\mu^2, \qquad \hat{p}_\mu = \frac{2}{a}\sin(\frac{ap_\mu}{2}). \tag{2.46}$$

[2] I acknowledge a very useful discussion with G.C. Rossi on this point.

The poles of the propagator give us the spectrum of the theory. If we now make an expansion for small lattice spacing a neglecting all the terms of $\mathrm{O}(a^2)$ we obtain

$$p^2 + m_0^2 + a m_0 r p^2 + \mu_{\mathrm{q}}^2, \qquad \text{where} \quad p^2 = p_\mu p_\mu. \tag{2.47}$$

The leading $\mathrm{O}(a)$ discretization effects of the dispersion relation are given by the term $a m_0 r p^2$. We can already make some interesting remarks. This term vanishes if we set $m_0 = 0$. This means that the chiral limit of the plain Wilson theory ($\mu_{\mathrm{q}} = 0$) does not have $\mathrm{O}(a)$ effects. Of course we are only considering the tree-level and if we would switch on the interaction the dynamics of the theory could change this result. We will see that if we consider the theory in a finite volume with suitable boundary conditions, where the mass dependence of the theory is smooth and there are no phase transitions, this result is still true.

From eq. (2.47) we also see that even if we set $m_0 = 0$ we can add a mass to the theory without introducing $\mathrm{O}(a)$ effects. To understand how this can happen it is good to understand the origin of the $\mathrm{O}(a)$ term $a m_0 r p^2$. It comes from the cross term between the Wilson term and the mass term in $\mathcal{M}(p)$. This cross term is absent with a twisted mass because twisted mass and Wilson term point in different "directions" in the chiral-flavour space.

Even if m_0 does not vanish but $m_0 = \mathrm{O}(a)$ this will not change our conclusion since the term with m_0 will only change the $\mathrm{O}(a^2)$ terms.

All these considerations are only at tree-level, but we will see in sect. 4 that they remain true if we switch on the interaction between quarks and gluons. In particular setting the Wtm action at full twist allows to have physical observables that are automatically $\mathrm{O}(a)$ improved.

2.6 Transfer matrix

Necessary and sufficient conditions under which the physical content of the theory in Minkowski space can be reconstructed from Euclidean Green's functions are the so called Osterwalder-Schrader conditions [26, 27]. One of the required properties that does not obviously hold in a lattice theory is physical positivity. This condition states that given a gauge invariant polynomial of positive time ($x_0 > 0$) fundamental fields O one should have

$$\langle \Theta(O^\dagger) O \rangle \geq 0 \tag{2.48}$$

where Θ denotes euclidean time reflection and $O^\dagger$ is the Hermitian conjugate of O. An explicit expression for the transfer matrix that in particular is strictly positive, i.e. all its eigenvalues are bigger than zero, was given for Wilson fermion and gauge actions in ref. [28]. This allows to prove the positivity condition (2.48) for the Wilson

action at finite lattice spacing.

In the app. C we briefly repeat the steps of the proof with the extension to Wtm, because they become important for non-degenerate quarks. Here we simply list the main result: adding a twisted mass term for degenerate quarks does not change [29] the constraint on κ ($|\kappa| < \frac{1}{6}$) valid [28] for Wilson fermions.

2.7 Renormalization

In perturbation theory, it has been shown that Wilson lattice QCD is renormalizable [30–34], and we shall assume that this remains true beyond perturbation theory. Since the twisted mass term can be viewed as a super-renormalizable interaction term which does not modify the power counting, this result can be extended also to Wtm.

To understand the structure of the counterterms we use the symmetries of the Wtm lattice action (2.28), treating the masses as spurion fields which transform under these symmetries. The counterterms to the action with dimension less or equal four are

$$\mathrm{tr}\{F_{\mu\nu}F_{\mu\nu}\}, \quad \overline{\chi}\chi, \quad m_0\overline{\chi}\chi, \quad i\mu_{\mathrm{q}}\overline{\chi}\gamma_5\tau^3\chi, \tag{2.49}$$

where $F_{\mu\nu}$ is the gluon field strength tensor. The first counterterm gives a multiplicative renormalization of the bare gauge coupling. The others enter in the renormalization of the bare quark masses. The continuum renormalized quark action can then be written as

$$S_0 = S_G[A] + \int d^4x\overline{\chi}(x)\Big[\gamma_\mu D_\mu + m_{\mathrm{R}} + i\mu_{\mathrm{R}}\gamma_5\tau^3\Big]\chi(x), \tag{2.50}$$

where S_G now is the continuum gluon action. The renormalized parameters are given by

$$g_{\mathrm{R}}^2 = g_0^2 Z_{\mathrm{g}}(g_0^2, a\mu), \tag{2.51}$$

$$m_{\mathrm{R}} = m_q Z_{\mathrm{m}}(g_0^2, a\mu), \tag{2.52}$$

$$\mu_{\mathrm{R}} = \mu_{\mathrm{q}} Z_\mu(g_0^2, a\mu), \tag{2.53}$$

where μ denotes the renormalization scale dependence of the renormalization constants Z, and

$$m_q = m_0 - m_{\mathrm{cr}}. \tag{2.54}$$

It is well known that due to the loss of chiral symmetry at finite lattice spacing, the bare untwisted quark mass renormalizes also additively, with a linearly divergent (with the lattice spacing) counterterm m_{cr}. The critical line m_{cr} is the value of m_0 where the untwisted quark mass vanishes. We will extensively discuss in sect. 4.3 how to define non-perturbatively the critical mass. For the moment we just assume

that such a value exists. Because of the $\widetilde{\mathcal{P}}$ symmetry defined in eq. (2.39) the flavour-parity violating operator $\overline{\chi}\gamma_5\tau^3\chi$ comes with a coefficient odd in $\mu_{\rm q}$, and opposite to what happens to the untwisted quark mass, the twisted mass is renormalized only multiplicatively. To state it differently, for zero twisted mass, parity is a symmetry of the bare action. The residual $U_{\rm V}(1)_3$ symmetry (2.40) forbids bilinears containing flavour matrices $\tau^{1,2}$, and the parity flavour symmetry $\mathcal{P}_F^{1,2}$ requires that parity and flavour are violated together, so it forbids flavour singlet parity violating terms $\overline{\chi}\gamma_5\chi$ and $\epsilon_{\mu\nu\rho\sigma}F_{\mu\nu}F_{\rho\sigma}$, as well as the flavour violating, parity even, operator $\overline{\chi}\tau_3\chi$. It is easy to check that all the dimension four operators which violate parity or isospin or both are ruled out by $\mathcal{P}_F^{1,2}$. The final continuum theory (2.50) has now only an apparent flavour and parity breaking. As we have already explained in sect. 2.2, provided that all the renormalization constants are defined in a mass independent scheme, this theory is equivalent to standard $N_{\rm f} = 2$ degenerate flavours QCD with a mass $M = \sqrt{m_{\rm R}^2 + \mu_{\rm R}^2}$, and no parity-flavour breaking.

2.8 Correlation functions

In sects. 2.1 and 2.2 we have seen that both in the classical theory, and in the quantum theory regularized in a chiral invariant way, there is an exact equivalence between QCD and tmQCD. This equivalence reflects itself in a correspondence between correlation functions computed in the two theories. In particular eq. (2.23) shows the relation between correlators, valid in the bare lattice theory regularized with GW fermions. Based on universality arguments we expect this equivalence to be true also with Wtm fermions between renormalized correlation functions.

The equations which relate correlation functions in the two theories depend on how the twist angle is defined. The twist angle can be defined in the renormalized theory, analogously to the continuum theory, by

$$\tan\omega = \frac{\mu_{\rm R}}{m_{\rm R}} = \frac{Z_\mu}{Z_{\rm m}}\frac{\mu_{\rm q}}{m_0 - m_{\rm cr}}. \tag{2.55}$$

To tune the twist angle it is then necessary to compute the ratio of renormalization constants $\frac{Z_\mu}{Z_{\rm m}}$ and the critical mass $m_{\rm cr}$. We will discuss extensively in sect. 4.3 how practically to determine the critical mass. One possible way to determine the critical mass is using the PCAC relation

$$m_{\rm R} = \frac{Z_A}{Z_P} m_{\rm PCAC} \quad \text{with} \quad m_{\rm PCAC} = \frac{\langle \partial_0 A_0^a(x) P^a(0)\rangle}{2\langle P^a(x) P^a(0)\rangle} \qquad a = 1, 2. \tag{2.56}$$

Measuring directly the PCAC mass, the twist angle is obtained by

$$\tan\omega = \frac{\mu_{\rm q}}{Z_A m_{\rm PCAC}}, \tag{2.57}$$

where we have used the fact, implied by the PCVC (7.2), that $Z_P = 1/Z_\mu$.

To tune the twist angle to $\omega = \pi/2$ it is not necessary to determine any renormalization constant, but only the critical mass.

Now that we have renormalized the theory in a mass independent scheme and we have determined the twist angle, using universality arguments, we can conclude that the relation between correlation functions in QCD and tmQCD can be inferred by the transformation of the integration variables (2.6), i.e.

$$\langle \mathcal{O}[\psi, \overline{\psi}] \rangle_{(M_{\rm R},0)} = \langle O[\chi, \overline{\chi}] \rangle_{(m_{\rm R},\mu_{\rm R})} \tag{2.58}$$

and at finite lattice spacing is valid up to cutoff effects. The index of the correlation function in the l.h.s indicates that it has been computed in standard QCD with renormalized quark mass $M_{\rm R}$ and $\mu_{\rm R} = 0$, and the index of the correlation function in the r.h.s indicates that it has been computed in tmQCD with renormalized quark masses $m_{\rm R}$ and $\mu_{\rm R}$ satisfying

$$M_{\rm R}^2 = m_{\rm R}^2 + \mu_{\rm R}^2. \tag{2.59}$$

Hence a given standard correlation function in QCD can be written as a linear combination of correlation functions computed in tmQCD at a given twist ω.

To summarize the procedure:

- start with the QCD correlation function you are interested in;
- perform the axial rotation that in the continuum brings the action from the physical basis to the twisted basis (see eq. (2.6)) on the fields appearing in the correlation function;
- compute the resulting correlation function with the Wtm lattice action in the twisted basis, with a choice of quark masses;
- perform the continuum limit.

The final result will be exactly the desired QCD correlation function in the continuum with quark mass $M_{\rm R}$ given by eq. (2.59).

We give here an explicit example, which is relevant for the extraction of the pseudoscalar decay constants and will be analyzed again in sect. 7.1.

The pion decay constant f_π can be determined in the standard Wilson case from the correlation function

$$\langle (\mathcal{A}_{\rm R})^1_0(x) P^1_{\rm R}(y) \rangle_{(M_{\rm R},0)}. \tag{2.60}$$

With Wilson fermions the axial current is not protected by chiral symmetry, hence it needs to be renormalized by the scale independent renormalization constant Z_A, which has to be determined to extract the decay constant from (2.60). If we want

to compute the same correlation function in tmQCD we perform first the axial rotation (2.6) on the fermion fields in (2.60), obtaining

$$\langle (\mathcal{A}_{\rm R})^1_0(x) P^1_{\rm R}(y)\rangle_{(M_{\rm R},0)} = \cos(\omega)\langle (A_{\rm R})^1_0(x) P^1_{\rm R}(y)\rangle_{(m_{\rm R},\mu_{\rm R})} + \sin(\omega)\langle (V_{\rm R})^2_0(x) P^1_{\rm R}(y)\rangle_{(m_{\rm R},\mu_{\rm R})}. \tag{2.61}$$

This relation is very useful because, as we will see in sect. 7.1, there is a definition of the vector current which is protected from any renormalization. As a consequence at $\omega = \pi/2$, the decay constant can be computed with Wtm without the computation of any renormalization constant.

2.9 Exceptional configurations

One of the historical reasons why a twisted mass term was introduced is the so called problem of exceptional configurations that we are briefly going to explain.

We have seen that lattice QCD with Wilson quarks [1] breaks explicitly chiral symmetry. To deal with this breaking we have to add suitable counterterms [35] in order to restore chiral symmetry in the continuum limit. We have seen, e.g., in sect. 2.7, that the ordinary untwisted quark mass is renormalized also additively. As a consequence the value of m_0 which corresponds to physical light quark masses is typically negative. This could have further practical consequences. In fact it implies that the Wilson-Dirac operator is not protected against zero modes. The Wilson operator $D_{\rm W}$ (2.29) fulfills the property $\gamma_5 D_{\rm W}\gamma_5 = D^\dagger_{\rm W}$. We can then define the Hermitian Wilson operator

$$Q_W \equiv \gamma_5(D_{\rm W} + m_0) \quad Q_W = Q^\dagger_W. \tag{2.62}$$

Q_W can have in general, for a given gauge configuration, a very small eigenvalue, even at values of m_0 which correspond to a not so small quark mass. These modes are expected to disappear in the continuum limit, but they can still be dangerous in numerical simulations

To understand this we write a pseudoscalar density propagator

$$C_P(x) = -\langle \overline{\psi}(x)\gamma_5 \frac{\tau^1}{2}\psi(x)\overline{\psi}(0)\gamma_5\frac{\tau^1}{2}\psi(0)\rangle \tag{2.63}$$

in terms of eigenfunctions and eigenvalues of Q_W. Performing the functional integral (see eq. 2.21) over the fermion fields we obtain

$$C_P(x) = \frac{1}{2}\mathcal{Z}^{-1}\int D[U]\ \det(Q^2_W){\rm tr}\left[Q^{-1}_W(0,x)Q^{-1}_W(x,0)\right]{\rm e}^{-S_G}, \tag{2.64}$$

This example shows the well-known fact that a functional integral over Grassmann variables cannot diverge. In fact if we write the the r.h.s of eq. (2.64) in terms of

eigenfunctions $\phi_i(x)$ and eigenvalues λ_i of Q_W we obtain [3]

$$C_P(x) \propto \int D[U] \left[\prod_i \lambda_i^2\right] \sum_{j,k} \phi_j(0) \frac{1}{\lambda_j} \phi_j^*(x) \phi_k(x) \frac{1}{\lambda_k} \phi_k^*(0). \tag{2.65}$$

After integration over the quark fields, a small eigenvalue of the Wilson operator appears both in the fermionic determinant and in the quark propagators entering the correlation functions. If a small eigenvalue occurs in the course of the integration over the gauge fields, the contributions from the denominators are always exactly compensated by the same eigenvalues in the expression for the determinant.

A problem arises however in the so-called quenched model, which consists in neglecting the fermionic determinant. The contribution of a small eigenvalue to a fermionic correlator is then not balanced by the determinant, leading to large fluctuations in some of the observables which completely compromise the ensemble average. Gauge field configurations where this happens are called "exceptional". The approach to the chiral limit in the quenched model with ordinary Wilson quarks is then limited by exceptional configurations.

In refs. [36,37], to solve the problem of exceptional configurations, was suggested to perform a chiral rotation of the mass term. But in ref. [36] was suggested to send the twisted mass to zero at the end of the computation, i.e. treating the twisted mass as an external source not as the real mass term, and in both references the axial rotation was anomalous, i.e. flavour singlet. Hence it would have not been possible to use it as an alternativ discretization of lattice QCD.

Adding the twisted mass term (2.28) to the Wilson action solves in a straightforward way the problem [15]. For the 2 flavours Wtm operator $D = D_W + m_0 + i\mu_{\rm q}\gamma_5\tau^3$ we have

$$Q = \gamma_5 D = Q_W + i\mu_{\rm q}\tau^3 \Rightarrow Q^\dagger Q = Q_W^\dagger Q_W + \mu_{\rm q}^2 = Q_W^2 + \mu_{\rm q}^2 \ . \tag{2.66}$$

This means that the Wtm operator does not have exceptionally small eigenvalues for arbitrary gauge fields: they can only appear in the massless ($\mu_{\rm q} = 0$) theory.

These considerations are true if we assume that the distribution of the eigenvalues of Q_W are either mass independent (like in the quenched model) or the mass dependence is analytic near the chiral point. We will see in sect. 6 that in infinite volume this is not true because of the non trivial chiral phase structure for Wilson fermions. On the contrary, approaching the chiral limit at fixed finite volume could in principle be advantageous using Wtm.

[3] Strictly speaking we are working in a finite volume where the spectrum of Q_W is discrete. This is practically the case in all the numerical simulations.

3 Non-degenerate quarks

In this section we show how twisted mass QCD can be generalized to a doublet of non-degenerate quarks. We extend the topics covered in the previous section to the non-degenerate case, emphasizing the main differences with the degenerate case.

3.1 Continuum actions

The continuum action we have discussed in sect. 2.1 describes two degenerate light quarks. To add a further doublet of non-degenerate quarks in order to describe the heavier (c,s) quarks, two proposals have been made [38, 39]. Both proposals can of course be used to describe a possible non-degeneracy also in the light sector. The first proposal [38] is based on a flavour off-diagonal splitting

$$S_{\rm F}[\chi,\overline{\chi},G] = \int {\rm d}^4x\, \overline{\chi}\left(\gamma_\mu D_\mu + m_{\rm q} + i\mu_{\rm q}\gamma_5\tau^3 + \epsilon_{\rm q}\tau^1\right)\chi, \tag{3.1}$$

where we take $\mu_{\rm q} > 0$ and $\epsilon_{\rm q} > 0$. The off-diagonal splitting is particularly interesting because, as we will see, it retains all the nice properties of tmQCD at full twist and it keeps the quark determinant real and positive if $\sqrt{m_{\rm q}^2+\mu_{\rm q}^2} > \epsilon_{\rm q}$ (see below and sect. 3.2).

In order to change from the *twisted basis* to the *physical basis* the following field transformations are needed. First we need an isovector rotation of $\omega_2 = \pi/2$

$$\chi' = \exp(i\omega_2\tau^2/2)\chi|_{\omega_2=\pi/2} = \frac{1}{\sqrt{2}}(1+i\tau^2)\chi, \tag{3.2}$$

$$\overline{\chi}' = \overline{\chi}\exp(-i\omega_2\tau^2/2)|_{\omega_2=\pi/2} = \overline{\chi}\frac{1}{\sqrt{2}}(1-i\tau^2). \tag{3.3}$$

This vector transformation leaves invariant the kinetic term and transforms the mass terms as

$$m_q + i\mu_q\gamma_5\tau^3 + \epsilon_q\tau^1 \to m_q - i\mu_q\gamma_5\tau^1 + \epsilon_q\tau^3. \tag{3.4}$$

Now we perform an axial rotation as before in the direction of the twisted mass term

$$\psi = \exp(-i\omega_1\gamma_5\tau^1/2)\chi', \qquad \overline{\psi} = \overline{\chi}'\exp(-i\omega_1\gamma_5\tau^1/2). \tag{3.5}$$

This transformation leaves the form of the action invariant, but transforms only the mass term with $\mu_{\rm q}$, and, if we want to have the standard action, the rotation angle ω_1 has to satisfy eq. (2.9). The action now looks like

$$S_{\rm F}[\psi,\overline{\psi}] = \int {\rm d}^4x\, \overline{\psi}\left(\gamma_\mu D_\mu + M + \epsilon_{\rm q}\tau^3\right)\psi, \tag{3.6}$$

where $M = \sqrt{m_q^2 + \mu_q^2}$ is again the polar mass. We remark here that these are the transformations needed given the action in eq. (3.1). Choosing a different basis for the action one is interested in (typically depending on the details of the lattice simulations), will induce different field transformations in order to connect the initial basis with the physical one.

Analogously to the degenerate case we can derive the partial conservation laws

$$\partial_\mu A_\mu^a = 2m_{\rm q} P^a + i\mu_{\rm q}\delta^{3a} S^0 + \epsilon_{\rm q}\delta^{a1} P^0, \tag{3.7}$$

$$\partial_\mu V_\mu^a = -2\mu_{\rm q}\,\varepsilon^{3ab} P^b + i\epsilon_{\rm q}\varepsilon^{1ab} S^b, \tag{3.8}$$

where

$$P^0 = \overline{\chi}\gamma_5\chi, \qquad S^a = \overline{\chi}\frac{\tau^a}{2}\chi. \tag{3.9}$$

If we have in mind to describe with this action the heavy doublet (c,s) we will naturally associate the quark mass in the following way:

$$m_c = M + \epsilon_q \qquad m_s = M - \epsilon_q. \tag{3.10}$$

The fermion determinant will then be positive if $M > \epsilon_{\rm q}$. This constraint will be reconsidered when introducing the Wilson term in the lattice actions, and taking into account how the bare masses are renormalized.

Another way to extend the tmQCD action to four flavours has been proposed in ref. [39]. In this proposal the continuum action reads

$$S_{\rm F}[\chi,\overline{\chi},G] = \int {\rm d}^4x\,\overline{\chi}\,(\gamma_\mu D_\mu + \mathbf{m} + i\boldsymbol{\mu}\gamma_5)\,\chi, \tag{3.11}$$

where now χ collects four quark fields $\chi^T = (u,d,s,c)$ and the mass matrices have the form

$$\mathbf{m} = \begin{pmatrix} m_u & 0 & 0 & 0 \\ 0 & m_d & 0 & 0 \\ 0 & 0 & m_s & 0 \\ 0 & 0 & 0 & m_c \end{pmatrix} = \begin{pmatrix} M_u\cos\omega_l & 0 & 0 & 0 \\ 0 & M_d\cos\omega_l & 0 & 0 \\ 0 & 0 & M_s\cos\omega_h & 0 \\ 0 & 0 & 0 & M_c\cos\omega_h \end{pmatrix}, \tag{3.12}$$

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_u & 0 & 0 & 0 \\ 0 & \mu_d & 0 & 0 \\ 0 & 0 & \mu_s & 0 \\ 0 & 0 & 0 & \mu_c \end{pmatrix} = \begin{pmatrix} M_u\sin\omega_l & 0 & 0 & 0 \\ 0 & -M_d\sin\omega_l & 0 & 0 \\ 0 & 0 & M_s\sin\omega_h & 0 \\ 0 & 0 & 0 & -M_c\sin\omega_h \end{pmatrix}, \tag{3.13}$$

Hence the theory has six independent parameters, namely the four polar quark masses M_i ($i = u,d,s,c$), with $M_i^2 = m_i^2 + \mu_i^2$, and the two twist angles ω_l, ω_h.

In other words, the four standard mass parameters m_i and the four twisted mass parameters μ_i are constrained by

$$\tan\omega_l = \frac{\mu_u}{m_u} = -\frac{\mu_d}{m_d}, \qquad \tan\omega_h = \frac{\mu_s}{m_s} = -\frac{\mu_c}{m_c}. \tag{3.14}$$

This framework extends the degenerate two-flavour tmQCD to non-degenerate quarks with the property that the quark mass terms remain flavour diagonal. At vanishing twist angles ω_l and ω_h one recovers the standard QCD action of four quark flavours, while for $\omega_h = 0$ and $M_u = M_d$ the two-flavour version of tmQCD in eq. (2.1) is reproduced, with two additional untwisted quark flavours s and c.

Given the form of the mass matrices (3.12,3.13) the rotation that has to be performed to go back to the *physical basis* is

$$\chi = \exp(-i\omega_l\gamma_5\tau_l^3/2 - i\omega_h\gamma_5\tau_h^3/2)\psi, \qquad \overline{\chi} = \overline{\psi}\exp(-i\omega_l\gamma_5\tau_l^3/2 - i\omega_h\gamma_5\tau_h^3/2), \tag{3.15}$$

with

$$\tau_l^3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad \tau_h^3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

and ω_l and ω_h satisfying eqs. (3.14). The four flavour QCD action now takes the standard form

$$S_{\rm F}[\psi,\overline{\psi},G] = \sum_{i=u,d,s,c}\int {\rm d}^4x\,\overline{\psi}_i(x)\left(\gamma_\mu D_\mu + M_i\right)\psi_i(x). \tag{3.16}$$

The rotation in eq. (3.15) will also give the relations among local fields in the 2 basis.

For a generic four flavour QCD theory with non-degenerate quarks, chiral and flavour symmetries are broken explicitly and this is expressed by the PCAC and PCVC relations (for $i \neq j$)

$$\partial_\mu A_{\mu,ij} = (m_i + m_j)P_{ij} + i(\mu_i + \mu_j)S_{ij}, \tag{3.17}$$

$$\partial_\mu V_{\mu,ij} = (m_i - m_j)S_{ij} + i(\mu_i - \mu_j)P_{ij}, \tag{3.18}$$

where the bilinear fields are defined by

$$S_{ij} = \overline{\chi}_i\chi_j, \quad P_{ij} = \overline{\chi}_i\gamma_5\chi_j, \quad A_{\mu,ij} = \overline{\chi}_i\gamma_\mu\gamma_5\chi_j, \quad V_{\mu,ij} = \overline{\chi}_i\gamma_\mu\chi_j. \tag{3.19}$$

We can now write also the fermionic action proposed in ref. [38] for two non-degenerate quarks in the *twisted basis*

$$S_{\rm F}[\chi,\overline{\chi},U] = a^4 \sum_x \overline{\chi}(x)\Big[D_{\rm W} + m_0 + i\mu_{\rm q}\gamma_5\tau^3 + \epsilon_{\rm q}\tau^1\Big]\chi(x), \tag{3.20}$$

The introduction of the off-diagonal splitting leaves intact, for example, the symmetries $\widetilde{\mathcal{P}}$ and $\mathcal{P}^1_F$, while $\mathcal{P}^2_F$ is a symmetry only if combined with a sign change of $\epsilon_{\rm q}$

$$\widetilde{\mathcal{P}}^2_F \equiv \mathcal{P}^2_F \times [\epsilon_{\rm q} \to -\epsilon_{\rm q}]\,. \tag{3.21}$$

In sect. 3.1 we have argued that the determinant is always real and positive provided the constraint $\mu_{\rm q} > \epsilon_{\rm q}$ is fulfilled [4]. This is an important practical issue in order to perform dynamical simulations with the currently available algorithms, since the fermionic determinant is usually included with the gauge action to form an effective Boltzmann weight (see sect. 8 for a discussion on recent algorithmic developments).

To understand how the condition on the bare masses translates to the quantum theory, we anticipate here that the renormalization factors of $\mu_{\rm q}$ and $\epsilon_{\rm q}$ are related to the renormalization factors of the pseudoscalar and scalar currents, i.e.

$$\mu_{\rm R} = Z_{\rm P}^{-1}\mu_{\rm q}, \qquad \epsilon_{\rm R} = Z_{\rm S}^{-1}\epsilon_{\rm q}. \tag{3.22}$$

It is then easy to show that the constraint $\mu_{\rm q} > \epsilon_{\rm q}$ augmented with the definitions (3.22) gives

$$\frac{Z_{\rm P}}{Z_{\rm S}} > \frac{(\mu_{\rm c})_{\rm R} - (\mu_{\rm s})_{\rm R}}{(\mu_{\rm c})_{\rm R} + (\mu_{\rm s})_{\rm R}}, \tag{3.23}$$

where, having in mind phenomenological applications, we have defined

$$(\mu_{\rm c})_{\rm R} = \mu_{\rm R} + \epsilon_{\rm R}, \qquad (\mu_{\rm s})_{\rm R} = \mu_{\rm R} - \epsilon_{\rm R}. \tag{3.24}$$

To give an example, fixing the values of the renormalized *strange* and *charm* quark masses, gives the following constraints

$$(\mu_{\rm c})_{\rm R} \simeq 1.5{\rm GeV} \qquad (\mu_{\rm s})_{\rm R} \simeq 0.1{\rm GeV} \Rightarrow \frac{Z_{\rm P}}{Z_{\rm S}} \gtrsim 0.875. \tag{3.25}$$

The fermionic action proposed in ref. [39] for four non-degenerate flavours reads

$$S_{\rm F}[\chi,\overline{\chi},U] = a^4 \sum_x \overline{\chi}(x)\Big[D_{\rm W} + \mathbf{m} + i\boldsymbol{\mu}\gamma_5\Big]\chi(x), \tag{3.26}$$

[4] For simplicity we consider here the full twist case.

with $\chi^T = (u, d, s, c)$, $\mathbf{m}$ and $\boldsymbol{\mu}$ defined in eqs. (3.12,3.13). To discuss the properties of the fermionic determinant with the action (3.26) we assume that the light doublet is mass degenerate,

$$m_u = m_d = m_l, \qquad \mu_u = -\mu_d = \mu_l. \tag{3.27}$$

Then the integration over the light fermion fields yields to

$$\det_{N_f=2} \left[(D_W + m_l)\, \mathbb{1} + i\mu_l \gamma_5 \tau^3 \right] = \det_{N_f=1} \left[(D_W + m_l)^\dagger (D_W + m_l) + \mu_l^2 \right], \tag{3.28}$$

where the indices indicate in which flavour space the determinant is taken [15]. Hence the determinant of the light doublet is positive at non-zero μ_l, irrespective of the background gauge field. Integrating over strange and charm quarks one obtains

$$\det_{N_f=1} \left[(D_W + m_s)^\dagger (D_W + m_c) - \mu_s \mu_c + i\mu_c \gamma_5 (D_W + m_s) + i\mu_s \gamma_5 (D_W + m_c) \right], \tag{3.29}$$

which is real and positive only for degenerate strange and charm quarks. The other possibility 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. Even if in this case the positivity of the determinant is not guaranteed, recent numerical results [40] indicate that this is indeed the case.

Practically, with the action (3.26), there are two options: do not include the strange and the charm quarks in the determinant, or include them but without twist. The first option would correspond to a partially quenched simulation with $N_f = 2$ light dynamical quarks, i.e. the strange and the charm would remain quenched. The second option would correspond to a $N_f = 3, 4$ dynamical simulation with two light twisted quarks and two heavier non-degenerate untwisted quarks.

3.3 Transfer matrix

In sect. 2.6 we have seen that provided $|\kappa| < \frac{1}{6}$ Wtm fulfills physical positivity. In app. C we briefly repeat the steps of the proof with the extension to Wtm, because they are important for non-degenerate quarks.

In fact in app. C we show that if we add a non-degenerate doublet as in eq. (3.20) the constraint on κ has to be changed into

$$|\kappa| < \frac{1}{6 + 2a\epsilon_{\mathrm{q}}}, \qquad \epsilon_{\mathrm{q}} > 0. \tag{3.30}$$

This difference can be understood by the different Hermiticity property of the twisted mass term $i\mu_{\mathrm{q}}\gamma_5\tau^3$ and the splitting term $\epsilon_{\mathrm{q}}\tau^1$.

First simulations with non-degenerate twisted quarks [41] indicate that suitable values of $\epsilon_{\rm q}$ are rather small and since, in the continuum limit and for a value of the untwisted bare quark mass close to the critical mass, κ is near 1/8, for practical purposes the constraint (3.30) should not cause any limitation.

To conclude Wtm, like the pure Wilson theory, is reflection positive for all the relevant values of the bare parameters.

3.4 Renormalization

Here we shortly discuss the structure of the counterterms for the non-degenerate action (3.20) and we refer to the original paper [39] for the counterterm structure of the action (3.26). The only additional counterterm to those in eq. (2.49) allowed by the lattice symmetries is

$$\epsilon_{\rm q}\overline{\chi}\tau^1\chi. \tag{3.31}$$

Because of the $\widetilde{\mathcal{P}}_F^2$ symmetry defined in eq. (3.21), the flavour violating operator $\overline{\chi}\tau^1\chi$ comes with a coefficient odd in $\epsilon_{\rm q}$, and the twisted mass splitting is renormalized only multiplicatively. All the dimension four operators which violate parity or isospin or both are absent because $\mathcal{P}_F^{1,2}$ are still symmetries when $\epsilon_{\rm q} = 0$. The dimension three operators that are absent in eqs. (2.49,3.31) are all ruled out by $\mathcal{P}_F^1$ symmetry, with the exception of $\overline{\chi}\gamma_5\tau^2\chi$ that is ruled out by charge conjugation $\mathcal{C}$ which is still a symmetry of the action (3.20). To conclude, the continuum renormalized quark action for non degenerate quarks is

$$S_0 = S_G[A] + \int d^4x\overline{\chi}(x)\Big[\gamma_\mu D_\mu + m_{\rm R} + i\mu_{\rm R}\gamma_5\tau^3 + \epsilon_{\rm R}\tau^1\Big]\chi(x), \tag{3.32}$$

where in addition to the degenerate case we just have to add

$$\epsilon_{\rm R} = \epsilon_{\rm q} Z_\epsilon(g_0^2, a\mu). \tag{3.33}$$

4 O(a) improvement

The continuum limit of lattice QCD is of fundamental importance to relate numerical simulations with experimental results. Practically to perform the continuum limit it is crucial to simulate at several values of the lattice spacing a, and it is also possible (and sometimes mandatory) to improve the rate of the discretization errors from a to a^2, using a suitable lattice QCD action. A possibility is to apply Symanzik's improvement program [3–5], where the O(a) cutoff effects in on-shell quantities are cancelled by adding local O(a) counterterms to the lattice action and to the composite fields of interest [6–10]. A technical difficulty is that the improvement coefficients multiplying these counterterms are not known a priori. An alternative is to use Wtm at full twist. By this we mean Wtm with bare parameters tuned in order to have in the continuum limit a vanishing untwisted quark mass. We will show that in this case physical observables will be automatically O(a) improved without the knowledge of any improvement coefficient. The only parameter tuning required is that of the bare untwisted quark mass to its critical value.

4.1 Symanzik expansion

The form of the unimproved lattice action is

$$S[\overline{\chi},\chi,U] = S_G[U] + S_F[\overline{\chi},\chi,U]\ . \tag{4.1}$$

In this section we will analyse the O(a) effects, so we leave unspecified the form of the gauge lattice action S_G, since it would only change the theory at O(a^2). S_F is the Wtm quark action defined in eq. (2.28), that we rewrite here for convenience

$$S_{\rm F}[\chi,\overline{\chi},U] = a^4\sum_x \overline{\chi}(x)\Big[D_{\rm W} + m_0 + i\mu_{\rm q}\gamma_5\tau^3\Big]\chi(x). \tag{4.2}$$

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

$$S_{\rm eff} = S_0 + aS_1 + a^2S_2 + \ldots \tag{4.3}$$

The key constraint is that each term of the Lagrangian has to be invariant under the symmetries of the regularized theory, i.e. the lattice theory. The leading term, S_0, is the action of the target continuum theory

$$S_0 = S_G[A] + \int d^4x\overline{\chi}(x)\Big[\gamma_\mu D_\mu + m_{\rm R} + i\mu_{\rm R}\gamma_5\tau^3\Big]\chi(x). \tag{4.4}$$

discussed already in sect. 2.7. The remaining operators S_k have to be interpreted as operator insertions in the continuum theory. The continuum theory can be defined

employing a lattice with spacing much smaller than a, or using a chiral invariant regularization that fulfills the Ginsparg-Wilson relation. The terms in the effective action are of the form

$$S_k = \int d^4y \mathcal{L}_k(y) \tag{4.5}$$

where the Lagrangians $\mathcal{L}_k(y)$ are linear combinations of local composite fields of dimension $4+k$.

Cutoff effects come also from the local composite fields one is interested in. A generic renormalized local gauge invariant field $\phi_R(x)$, constructed from quark and gluon fields on the lattice, is represented in the effective theory by an effective field of the form

$$\phi_{\text{eff}}(x) = \phi_0(x) + a\phi_1(x) + a^2\phi_2(x) + \dots \tag{4.6}$$

where the fields ϕ_k should have the appropriate dimension and should transform under symmetries as the lattice field.

All on-shell quantities in QCD can be extracted from correlation functions of local composite fields. These correlation functions are needed at non-zero physical distance. We take a generic connected lattice correlation function made of a multiplicatively renormalized multilocal field

$$G(x_1, \dots, x_n) = \langle \phi_R(x_1) \cdots \phi_R(x_n) \rangle \equiv \langle \Phi \rangle \tag{4.7}$$

and we always consider $x_1 \neq x_2 \neq \cdots \neq x_n$. In the effective theory up to order a it will be described by

$$\langle \Phi \rangle = \langle \Phi_0 \rangle_0 - a \int d^4y \langle \Phi_0 \mathcal{L}_1(y) \rangle_0 + a \langle \Phi_1 \rangle_0 + \mathrm{O}(a^2) \tag{4.8}$$

where the expectation values on the right hand side are to be taken in the continuum theory with action S_0 and

$$\langle \Phi_0 \rangle_0 \equiv \langle \phi_0(x_1) \cdot \cdots \cdot \phi_0(x_n) \rangle_0 \tag{4.9}$$

$$\langle \Phi_1 \rangle_0 \equiv \sum_{k=1}^{n} \langle \phi_0(x_1) \cdots \phi_1(x_k) \cdots \phi_0(x_n) \rangle_0 \tag{4.10}$$

The second term in the r.h.s. of eq. (4.8) develops potentially divergent contact terms whenever $y = x_k$. An important remark [9] is that these contact terms do not spoil the form of the expansion. Any contact term coming from $\phi_0(x)\mathcal{L}_1(y)$ when $y \to x$ will be given by an operator that has the same dimension and symmetry properties as $\phi_1(x)$. Since we leave the expression of ϕ_1 unspecified, the way used to subtract the divergence from the contact term will not change the form of eq. (4.8). The explicit a dependence in eq. (4.8) is not the full a dependence of the lattice correlation function: ϕ_1 and $\mathcal{L}_1(y)$ are linear combinations of fields, the coefficients of which depend on a logarithmically, as shown in perturbation theory [5]. Additional

O(a) effects can arise if one integrates the lattice correlation functions over short distances, and these cutoff effects will not be described by the effective theory. We remind here that this is not a crucial restriction since hadron masses and matrix elements are computed from correlation functions at non-zero distance. This remark is also important because it allows further simplifications in determining the set of operators $\mathcal{O}_i$ contributing to $\mathcal{L}_1$. In app. D, I briefly summarize how to construct $\mathcal{L}_1$ and I give as an example the operators contributing to ϕ_1 for the currents A^a_μ, V^a_μ and P^a.

The result of this analysis gives as the leading term of the effective Lagrangian

$$\mathcal{L}_1 = \sum_{i=1}^{5} c_i \mathcal{O}_i \tag{4.11}$$

where

$$\mathcal{O}_1 = i\overline{\chi}\sigma_{\mu\nu}F_{\mu\nu}\chi, \tag{4.12}$$

$$\mathcal{O}_2 = m_{\rm q}\mathrm{tr}\{F_{\mu\nu}F_{\mu\nu}\}, \tag{4.13}$$

$$\mathcal{O}_3 = m^2_{\rm q}\overline{\chi}\chi, \tag{4.14}$$

$$\mathcal{O}_4 = m_{\rm q}\mu_{\rm q} i\overline{\chi}\gamma_5\tau^3\chi, \tag{4.15}$$

$$\mathcal{O}_5 = \mu^2_{\rm q}\overline{\chi}\chi. \tag{4.16}$$

Now that we know the form of the leading corrections to the effective action we can add to the Wtm Lagrangian the suitable counterterms in order to remove the O(a) terms from the lattice action. This will be already enough to improve all the spectral quantities like the hadron masses. The counterterms to add to the Wtm action are

$$a^5 \sum_x \sum_{i=1}^{5} \hat{c}_i \hat{\mathcal{O}}_i \ , \tag{4.17}$$

where the fields $\hat{\mathcal{O}}_i$ will be some lattice representation of the continuum $\mathcal{O}_i$. In general the form of the lattice fields $\hat{\mathcal{O}}_i$ is not fixed because this amounts to change the O(a^2) terms of the theory. These discretization ambiguities allow to represent the gauge strength field and the local scalar density in the way they already appear in the Wtm action. The O(a) counterterms $\mathcal{O}_2$ to $\mathcal{O}_5$ amount then to a reparametrisation of the twisted and untwisted quark masses together with the reparametrisation of the bare coupling g_0. These reparametrisations are important if one chooses a mass independent renormalization scheme. We have seen in sect. 2 that it is important to make such a choice, in order to have equivalence between twisted mass and standard QCD correlation functions. We assume now that a mass-independent renormalization scheme has been chosen. The O(a) improved action, also called clover action, is given by

$$S_{\rm impr}[\overline{\chi},\chi,U] = S[\overline{\chi},\chi,U] + \delta S[\overline{\chi},\chi,U] \ , \tag{4.18}$$

$$\delta S[\overline{\chi},\chi,U] = a^5 \sum_x c_{\rm sw}\overline{\chi}(x)\frac{i}{4}\sigma_{\mu\nu}\hat{F}_{\mu\nu}(x)\chi(x) \ , \tag{4.19}$$

where $\hat{F}_{\mu\nu}$ is a lattice representation of the gluon field strength tensor and $c_{\rm sw}$ is the so-called Sheikholeslami-Wohlert parameter [7]. This parameter depends on the bare gauge coupling and all the details of the lattice action (but not on the quark masses) and has to be tuned in order to achieve on-shell O(a) improvement. To define, consistently with O(a) improvement and a mass independent renormalization scheme, the renormalized coupling and masses we have to define the theory around the chiral point. We have seen in sect. 2.7, in the renormalization procedure, that in the plane of the bare parameters the massless point is given by $(m_0,\mu_{\rm q}) = (m_{\rm cr},0)$ where the critical line $m_{\rm c}$ is the value of m_0 where the physical quark mass vanish. Then is natural to introduce the subtracted bare quark mass

$$m_{\rm q} = m_0 - m_{\rm cr} \tag{4.20}$$

and to define the renormalized O(a) improved masses and coupling constant as

$$g^2_{\rm R} = \tilde{g}^2_0 Z_{\rm g}(\tilde{g}^2_0, a\mu), \tag{4.21}$$

$$m_{\rm R} = \tilde{m}_q Z_{\rm m}(\tilde{g}^2_0, a\mu), \tag{4.22}$$

$$\mu_{\rm R} = \tilde{\mu}_{\rm q} Z_{\mu}(\tilde{g}^2_0, a\mu), \tag{4.23}$$

where μ denotes the renormalization scale dependence of the renormalization constants Z, and the improved bare parameters are given by

$$\tilde{g}^2_0 = g^2_0(1 + b_{\rm g} a m_{\rm q}), \tag{4.24}$$

$$\tilde{m}_q = m_q(1 + b_{\rm m} a m_{\rm q}) + \tilde{b}_{\rm m} a\mu^2_{\rm q}, \tag{4.25}$$

$$\tilde{\mu}_{\rm q} = \mu_{\rm q}(1 + b_\mu a m_{\rm q}) \ . \tag{4.26}$$

It easy to recognize the 4 terms which correspond in the effective theory to $\mathcal{O}_i$ with $i = 2,3,4,5$. To summarize, to achieve full O(a) improvement it is necessary to tune not only $c_{\rm sw}$, but also the b and $\tilde{b}$ parameters defined in eqs. (4.24-4.26), and the improvement coefficients related to the operators one is interested in. To be specific the renormalized O(a) improved axial current will look like

$$(A_{\rm R})^a_\mu = Z_{\rm A}(1 + b_{\rm A} a m_{\rm q})\Big[A^a_\mu + a c_{\rm A}\partial_\mu P^a + a\mu_q \tilde{b}_{\rm A}\epsilon^{3ab}V^b_\mu\Big] \ , \tag{4.27}$$

where we have eliminated the operator $(\mathcal{O}_8)^a_\mu$ (D.8) using the equations of motion. In principle all these improvement coefficients would need to be computed to have an O(a) improved evaluation of an hadronic matrix element including an axial current. At this point the introduction of a twisted mass has added the b_μ and $\tilde{b}_m$ parameters together with some $\tilde{b}$ parameters for the improved operators. Still the number of improvement coefficients needed to be computed even without twisted mass is not negligible, especially if one considers non-degenerate quarks [42]. There are two

technical remarks to make. The set of O(a) counterterms that have been introduced are slightly redundant [29]. This generic feature of tmQCD can be traced back to the equivalence of correlation functions of tmQCD and standard QCD in the continuum limit. O(a) improved Wtm is a one-parameter family of O(a) improved theories: one of the improvement coefficient can be chosen arbitrarily. The choice is usually to set $\tilde{b}_{\rm m} = -1/2$ because with this choice almost all the other improvement coefficients vanish at tree-level of perturbation theory. The second remark is to note that the case $m_{\rm R} = 0$ is particularly interesting. In the most general case this corresponds to $m_{\rm q}$ being an O(a) (see eq. 4.22), and in the spirit of O(a) improvement, where O(a^2) effects are neglected, from eqs. (4.24-4.26) we infer that one remains with only one parameter $\tilde{b}_{\rm m}$ and moreover mass dependent O(a) effects in the bare coupling are absent. Given also the remark of the redundancy of the improvement coefficients Wtm at full twist is O(a) improved just tuning the clover term and all the improvement coefficients needed to improve the local operators. The $\tilde{b}$ parameters are associated with opposite parity operators and it is in principle possible to get rid of them in a quantum mechanical analysis (we will come back to this topic in sect. 6). So implementing the standard O(a) Symanzik's improvement program with Wtm at full twist ($m_{\rm R} = 0$) is cheaper in the number of improvement coefficients to compute, with respect to standard Wilson fermions.

We will see in sec. 4.2 that the situation of full twist when $m_{\rm R} = 0$ is of capital importance, and it has tremendous consequence in the cutoff effects of correlation functions. It is already clear then that it becomes extremely important to discuss the way of practically implementing on the lattice the condition $m_{\rm R} = 0$.

Before discussing the consequences of working at full twist, I briefly summarize some numerical results obtained with Wtm adopting the Symanzik's improvement program just discussed.

4.1.1 Numerical tests

The Symanzik program requires the knowledge of a set of improvement coefficients, that we have just discussed. A first possibility is to compute them in perturbation theory. A one loop computation would leave physical observables with O(ag_0^4) discretization errors and if the gauge coupling (the lattice spacing) is small enough it is reasonable to hope that the quantity of interest will numerically scale with O(a^2) corrections. A further check could be to change by factors of O(1) the one loop improvement coefficients and check if the scaling violations change dramatically or not. A better approach is to compute the improvement coefficients non-perturbatively. Some of the improvement coefficients have been computed non-perturbatively, within the ordinary Wilson framework, both in the quenched model [43, 44], in the $N_f = 2$ [45] and in the $N_f = 3$ theory [46].

The improvement coefficients computed in a mass independent renormalization scheme do not depend on the form of the mass term and they can be used also with Wtm fermion. Only the additional improvement coefficients, specific to Wtm, need to be determined in addition. In [29] it has been shown how to implement the standard Symanzik program for Wtm, and many improvement coefficients have been computed at one loop in perturbation theory, especially the improvement coefficients related to Wtm.

One is certainly interested in checking numerically if the $\mathrm{O}(a)$ improvement has been successfully implemented and if the remaining $\mathrm{O}(a^2)$ effects are small. In particular quantities which have a finite continuum limit can be computed at several values of the lattice spacing to check the amount of *scaling violations*. In particular these scaling studies have to be performed on a line of constant physics. With this we mean that changing the lattice spacing the bare parameters have to be changed keeping a number of (physical) quantities, corresponding to the number of bare parameters, fixed.

In the quenched model it is standard to tune the quark mass keeping fixed an hadronic mass and to tune the gauge coupling keeping fixed the so called Sommer parameter r_0 [47]. r_0 is an intermediate distance (usually fixed to be 0.5 fm) where the force between two static quark is evaluated. While this quantity can be measured on the lattice very precisely, it has a rather uncertain phenomenological value. In the quenched model this is not a big problem, since the systematic error of neglecting the fermionic determinant is anyhow unknown, and the precise determination of the value of the lattice spacing allows very careful analysis of scaling violations. In the results presented here the values of r_0/a, where needed, are taken from [48].

A scaling test with $\mathrm{O}(a)$ improved Wtm has been performed [49] in the quenched model and in a finite volume $(L^3 \times T \simeq 0.75^3 \times 1.5)$ fm^4 with Schrödinger functional boundary conditions [50–52]. [5] The renormalized quark masses were fixed in such a way that the ratio of untwisted to twisted mass was [6]

$$\frac{m_{\mathrm{R}}}{\mu_{\mathrm{R}}} \simeq 0.131. \tag{4.28}$$

The outcome of the study is that even if some improvement coefficients are known only at one loop in perturbation theory, for lattice spacings $a \geq 0.093$ fm the scaling

[5] These boundary conditions allow to perform in intermediate volumes scaling studies of the lattice theory close to the continuum limit. In particular this framework allows very precise determinations of several quantities which have a well defined continuum limit and can be used to study scaling violations. Moreover these quantities become phenomenologically relevant in the infinite volume limit.

[6] It is interesting to note that in this study, even if the untwisted quark mass is small, we are not at full twist.

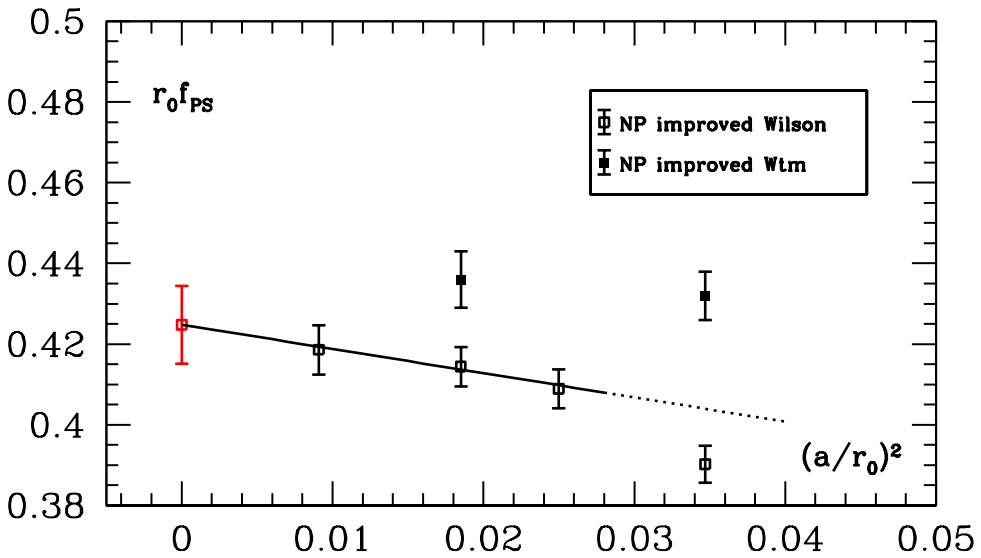


Fig. 1. $f_{\rm PS}$ vs. a^2 at at a fixed value of the pseudoscalar mass $M_{\rm PS} \simeq 1.2 M_{\rm K^\pm}$ for non-perturbatively (NP) improved Wilson fermions (□) [54] and non-perturbatively (NP) improved Wilson twisted mass (■) [53]. The continuum extrapolation by ref. [54] is also shown.

behaviour of some renormalized and improved quantities (which in large volume yield the mass and the decay constant of pseudoscalar and vector mesons) is consistent with O(a) improvement, with residual cutoff effects at $a = 0.093$ fm ranging from 0.5% to 9%.

The same setup and observables have then been employed for a study in large volumes [53]: $L = 1.5$ to 2.2 fm and $T = (2-3)L$. This study was restricted to two lattice resolutions, $a = 0.093$ and 0.068 fm, and, for each of them, three sets of quark mass parameters, which correspond to $|\omega| = \pi/2 + {\rm O}(a)$ and pseudoscalar meson masses $M_{\rm PS}$ in the range $1.85 \geq (M_{\rm PS}/M_{\rm K^\pm})^2 \geq 0.85$.

The scaling behaviour of the pseudoscalar decay constant $f_{\rm PS}$ in large volume is presented in fig. 1 for the O(a) improved Wilson formulations with $|\omega| \simeq \pi/2$ [53] (■) and $\omega = 0$ [54] (□). In the latter case four lattice resolutions were considered to allow for continuum extrapolation. The results for $f_{\rm PS}\, r_0$ that are obtained from the two lattice formulations should agree in the continuum limit: this seems to be the case within the statistical errors shown in the figures. It is very interesting to note that Wtm at full twist, for this physical quantity, shows a much weaker a^2 dependence compared with O(a) improved Wilson fermions.

4.2 Automatic O(a) improvement

We have shown that O(a) improved Wtm requires the computation of less improvement coefficients than Wilson fermions. In particular we have seen that setting Wtm at full twist only $c_{\rm sw}$ has to be computed in order to remove the O(a) from the action and from the reparametrisation of the quark masses and gauge coupling. While to improve operator matrix elements the standard improvement coefficients are needed. All the improvement coefficients depend on the details of the lattice action, in particular they depend for example on the choice of the gauge action or on the way it is discretized the lattice derivative.

In a remarkable paper of Frezzotti and Rossi [11] a step forward was made. It was proved that correlation functions made of parity even multiplicatively renormalizable fields are free from O(a) effects, and so no improvement coefficients are needed, if in the continuum limit $m_{\rm R} = 0$ (see eq. 4.4 and eq. 4.22), i.e. if the physical quark mass is given solely by the twisted mass $\mu_{\rm R}$.

We will call this property *automatic O(a) improvement*. The first remark is that the theory itself is not improved, but the physical correlation functions are. To say it in another way, from all the possible sets of correlation functions that define the regularized theory, the O(a) effects are all in those which vanish in the continuum limit. In particular the parity odd correlators, which vanish in the continuum limit, will have a first contribution of O(a) while the parity even correlators will have as a first correction to the continuum value an O(a^2) error.

4.2.1 Proof

Automatic O(a) improvement can be demonstrated in many ways, and many proofs appeared in the literature [11, 55–60]. The first proof was given in ref. [11], which is sketched in app. E. This proof is based on a set of spurionic symmetries of the lattice action.

Automatic O(a) improvement can be proved in a different way just considering the symmetries of the continuum action. In the following I try to summarize the proof which emphasize the role of the symmetries of the continuum action [57, 58], the automatic O(a) improvement of the massless Wilson operator in a finite volume [59], and the usage of symmetries which are not spontaneously broken in infinite volume continuum QCD [60].

Before going in details in the proof I would like to give an historical remark, in Minkowski space, that is not directly connected to twisted mass, but it helps to clarify the nature of the cutoff effects in the Wilson theory. The leading non-

renormalizable corrections to QED would be those interactions of dimension 5, which are suppressed by only one factor of $1/E$, where E is some high energy scale. According to Lorentz, gauge and $\mathcal{CP}$ invariance there is only one term allowed: the Pauli term proportional to $1/E\overline{\psi}\sigma_{\mu\nu}F^{\mu\nu}\psi$. The contribution of this term to the magnetic moment of the electron or muon would give a constraint on the value of E. It is well known, see for instance sec. 12.3 of [14], that this constraint can be strengthened using the following argument. The QED Lagrangian is symmetric under the following chiral transformation $\psi \to \gamma_5\psi$ and $m \to -m$, were m is the lepton mass. Then assuming that also the inclusion of a Pauli term should respect this symmetry we see immediately that the Pauli term in the Lagrangian would have to appear with an extra multiplicative factor m/E, i.e. $m/E^2\overline{\psi}\sigma_{\mu\nu}F^{\mu\nu}\psi$. We will see now that this is essentially the mechanism responsible for automatic O(a) improvement, because the Pauli term describes the leading discretization errors with an energy scale $E \sim 1/a$.

We first consider the massless Wtm action (eq. 2.28 with $m_0 = m_{\rm cr}$, $\mu_{\rm q} = 0$) in a finite volume with suitable boundary conditions for all the fields. The choice to work in a finite volume is done to keep the mass dependence smooth and avoid any complications with possible phase transitions.

The Symanzik effective action reads

$$S_{\rm eff} = S_0 + aS_1 + \ldots \tag{4.29}$$

and we are interested in a massless continuum target theory.

$$S_0 = \int d^4x \overline{\chi}(x)\Big[\gamma_\mu D_\mu\Big]\chi(x) \tag{4.30}$$

The correction terms in the effective action are given by

$$S_1 = \int d^4y \mathcal{L}_1(y) \qquad \mathcal{L}_1(y) = \sum_i c_i \mathcal{O}_i(y). \tag{4.31}$$

In the massless case the only operator contributing is

$$\mathcal{O}_1 = i\overline{\chi}\sigma_{\mu\nu}F_{\mu\nu}\chi, \tag{4.32}$$

which is the usual clover term. We consider now a general multiplicatively renormalizable multilocal field that in the effective theory is represented by the effective field

$$\Phi_{\rm eff} = \Phi_0 + a\Phi_1 + \ldots \tag{4.33}$$

A lattice correlation function of the field Φ to order a is given by

$$\langle\Phi\rangle = \langle\Phi_0\rangle_0 - a\int d^4y \langle\Phi_0\mathcal{L}_1(y)\rangle_0 + a\langle\Phi_1\rangle_0 + \ldots \tag{4.34}$$

where the expectation values on the r.h.s are to be taken in the continuum theory with action S_0. The key point is that the continuum action (4.30) is chirally symmetric, e.g. the following discrete chiral symmetry

$$\mathcal{R}_5^{1,2}: \begin{cases} \chi(x_0,\mathbf{x}) \to i\gamma_5\tau^{1,2}\chi(x_0,\mathbf{x}) \\ \overline{\chi}(x_0,\mathbf{x}) \to \overline{\chi}(x_0,\mathbf{x})i\gamma_5\tau^{1,2} \end{cases} \tag{4.35}$$

is a symmetry of the continuum action, while all the operators in eq. (4.32), of the Symanzik expansion of the lattice action, are odd under the discrete chiral symmetry $\mathcal{R}_5^{1,2}$ of the continuum action.[7] If the operator Φ is a lattice representation of the continuum chirally even field Φ_0, then the second term in the r.h.s. of eq. (4.34) vanishes. To show that also the Φ_1 term vanishes we have to show that an operator of one dimension higher than the original one but with the same lattice symmetries has opposite chirality. To do this we introduce a symmetry that essentially counts the dimensions of the operators [11]

$$\mathcal{D}: \begin{cases} U(x;\mu) \to U^\dagger(-x-a\hat{\mu};\mu), \\ \chi(x) \to \mathrm{e}^{3i\pi/2}\chi(-x) \\ \overline{\chi}(x) \to \overline{\chi}(-x)\mathrm{e}^{3i\pi/2}. \end{cases} \tag{4.36}$$

The gauge lattice action is invariant under $\mathcal{D}$ while in the fermion lattice action the terms that break chiral symmetry are odd. But in particular the lattice action is invariant under $\mathcal{R}_5^{1,2} \times \mathcal{D}$. So the operators in Φ_1 will necessarily have opposite chirality to Φ_0. Given the fact that the continuum action is chirally symmetric also Φ_1 vanishes. The conclusion is then: the chiral limit of the Wilson theory is automatically O(a) improved, if we stay in a finite volume where no symmetry can be spontaneously broken [59]. We remark that the case of the Schrödinger functional is different since there the standard boundary conditions [51, 52] break the chiral symmetry so automatic O(a) improvement does not apply[8].

We add now a standard mass term $m_{\mathrm{R}}\overline{\chi}(x)\chi(x)$ to the action (4.30). The dimension 5 operators contributing to $\mathcal{L}_1$ are now given by the operators in eqs. (4.12-4.14).

[7] Strictly speaking in the massless case the non trivial flavour structure of $\mathcal{R}_5^{1,2}$ it is not needed to prove automatic O(a) improvement. It will become necessary in the massive case.

[8] Chirally twisted boundary conditions [59] have been introduced in order to obtain a bulk automatic O(a) improvement, with remaining O(a) cutoff effects stemming solely from the boundaries.

All these operators are odd under the spurionic symmetry [9]

$$\widetilde{\mathcal{R}}_5^{1,2} \equiv \mathcal{R}_5^{1,2} \times (m_{\rm R} \to -m_{\rm R}) \tag{4.37}$$

while the continuum action is even under $\widetilde{\mathcal{R}}_5^{1,2}$. This does not mean that the insertions of these operators in the Symanzik expansion vanish, but since we are in finite volume where the mass dependence is smooth this means that the cutoff effects are all of the kind $\mathrm{O}(am_{\rm q})$.

It seems like a similar argument could be given in infinite volume. This indeed is not the case because of the spontaneous breaking of chiral symmetry. Now the quark mass dependence around the chiral limit does not need to be smooth and even if all the leading $\mathrm{O}(a)$ effects are odd in the quark mass because of the spurionic symmetry $\widetilde{\mathcal{R}}_5^{1,2}$, a possible non-analyticity in the quark mass can generate pure $\mathrm{O}(a)$ cutoff effects. [10] To say it differently, the insertion of chirally odd operators does not vanish in the chiral limit because of the spontaneous symmetry breaking of chiral symmetry.

To obtain automatic $\mathrm{O}(a)$ improvement in infinite volume including a mass term, we have to consider as a target continuum theory for the fermion fields

$$\int d^4x \overline{\chi}(x) \Big[\gamma_\mu D_\mu + i\mu_{\rm R}\gamma_5\tau^3 \Big] \chi(x), \tag{4.38}$$

where the physical mass is given by the twisted mass term. While in the massless case it is not possible to make a distinction between vector and axial symmetries, in the massive case one usually associates the symmetry broken by the mass term with the axial symmetry. In the following we will refer generically to chiral symmetry, the form of which will depend on the form of the mass term. We remind the reader that in the twisted basis the symmetry left unbroken by the mass term is the "twisted" vector symmetry (2.44), and the symmetry broken by the mass term is the "twisted" axial symmetry (2.44) (cf. sec. 2.4.1).

We can repeat the same steps done in the first proof adding in $\mathcal{L}_1$ the term

$$\mathcal{O}_5 = \mu_{\rm q}^2 \overline{\chi}\chi. \tag{4.39}$$

The reason to have the physical mass term fully given by the twisted mass is that the continuum action (4.38) is still invariant under the discrete symmetry $\mathcal{R}_5^{1,2}$, and

[9] Actually also the operators in eqs. (D.6) and (D.7), which are eliminated using the equations of motion, are odd under the spurionic symmetry $\widetilde{\mathcal{R}}_5^{1,2}$. This means that in principle the equation of motion are not really needed to eliminate them in the context of automatic $\mathrm{O}(a)$ improvement.

[10] A simple example is given by $a\,\mathrm{sign}(m_{\rm q})$ where the sign function is still odd under $m_{\rm q} \to -m_{\rm q}$ but it is non analytic in $m_{\rm q} = 0$.

if we now count the dimensions of the operators including the mass

$$\widetilde{\mathcal{D}} = \mathcal{D} \times [\mu_{\rm q} \to -\mu_{\rm q}] \tag{4.40}$$

then $\mathcal{R}_5^{1,2} \times \widetilde{\mathcal{D}}$ is also still a symmetry of the lattice action [60]. We can then conclude that the second term in the r.h.s. of eq. (4.34) vanishes, and Φ_1, being of one dimension higher, is odd under a $\mathcal{R}_5^{1,2}$ transformation: for the same reason the third term in the r.h.s of eq. (4.34) vanishes. Possible contact terms coming from the second term amount to a redefinition of Φ_1 as we have discussed in sec. 4.1, and so do not harm the proof.

The reason why now spontaneous breaking of chiral symmetry does not spoil the proof, is that the twisted mass term breaks chiral symmetry in an orthogonal direction compared to the breaking of the Wilson term. Spontaneous chiral symmetry breaking is in the chiral flavour direction of the mass term, while the Wilson term, and accordingly the relevant dimension five operators $\mathcal{O}_1$ and $\mathcal{O}_5$ are "orthogonal", so are not affected by spontaneous chiral symmetry breaking.

It is interesting to note that $\mathcal{R}_5^{1,2}$ corresponds to a discrete twisted "charged" vector transformation defined in eq. (2.42). The actual symmetry used to prove automatic O(a) improvement is what would correspond in the physical basis to the standard charged flavour symmetry which is well known not to be spontaneously broken in continuum QCD [61].

The same proof can be repeated identically using, instead of chiral symmetry, the twisted parity symmetry [57, 58]

$$\mathcal{P}_{\frac{\pi}{2}}: \begin{cases} U(x_0,\mathbf{x};0) \to U(x_0,-\mathbf{x};0), \quad U(x_0,\mathbf{x};k) \to U^{-1}(x_0,-\mathbf{x}-a\hat{k};k), \quad k=1,\,2,\,3 \\ \chi(x_0,\mathbf{x}) \to \gamma_0(i\gamma_5\tau^3)\chi(x_0,-\mathbf{x}) \\ \overline{\chi}(x_0,\mathbf{x}) \to \overline{\chi}(x_0,-\mathbf{x})(i\gamma_5\tau^3)\gamma_0, \end{cases} \tag{4.41}$$

which is also not spontaneously broken in continuum QCD [62]. The only difference would be that for matrix elements with non-vanishing momenta, the twisted parity proof requires, an average of matrix elements computed with momentum $\mathbf{p}$ and $-\mathbf{p}$, while this is not required using chiral symmetry. It is then clear that in order to achieve automatic O(a) improvement, the continuum target theory must have a vanishing untwisted quark mass $m_{\rm R}$, otherwise the standard mass term $m_{\rm R}\overline{\chi}\chi$ will break the residual "twisted" vector symmetry $\mathcal{R}_5^{1,2}$ (or the twisted parity symmetry $\mathcal{P}_{\frac{\pi}{2}}$) of the continuum action. The most natural way to achieve this on the lattice is by setting the untwisted bare quark mass to its critical value $m_0 = m_{\rm cr}$. The proof also shows that a possible uncertainty of O(a) in the critical mass does not invalidate automatic O(a) improvement since these uncertainties are odd under "twisted" vector symmetry (or twisted parity).

The careful reader may wonder what happens to automatic O(a) improvement if the critical mass is fixed such that the untwisted quark mass is of O(a). We recall that the theory itself it is not improved, but only the physical correlators are. In principle to obtain automatic O(a) improvement we have seen it is necessary to have $m_{\rm R} = 0$, only in the continuum limit, which means at finite lattice spacing at most $m_{\rm q} = {\rm O}(a)$ (see eq. (4.22,4.25)). This uncertainty can be described by a dimension 5 operator

$$\mathcal{O}_0 = \Lambda^2 \overline{\chi}\chi, \tag{4.42}$$

where Λ^2 is some energy scale squared which depends on the way the critical mass is determined, e.g. it could be of the order of the QCD scale $\Lambda^2_{\rm QCD}$, or it could be something proportional to $\Lambda_{\rm QCD}\mu_{\rm q}$. In particular to have a massless continuum theory in general we have $m_{\rm q} = {\rm O}(a)$. We can say that the operator $\mathcal{O}_0$ parameterizes O(a) uncertainties in the critical mass. This uncertainty does not harm automatic O(a) improvement because is described by an operator which is odd under the transformation $\mathcal{R}_5^{1,2}$ which is symmetry of the continuum action (4.38).

We can conclude that correlators which are even under a twisted parity or twisted vector transformation, are automatically O(a) improved without the knowledge of any improvement coefficient, and by just tuning the critical mass such that the untwisted quark mass is at most $m_{\rm q} = {\rm O}(a)$.

From the proof apparently there are no constraints on the values of the quark masses $\mu_{\rm q}$ where automatic O(a) improvement is at work. The presence of the Wilson term in the lattice action enforces us to perform a continuum limit first at a fixed value of the renormalized quark mass, and then to study the quark mass dependence, but it is important to understand how low we can go with the quark mass at fixed lattice spacing.

To have a first guess we can take the polar mass

$$M_{\rm R} = \sqrt{\mu_{\rm R}^2 + m_{\rm R}^2} = \sqrt{\mu_{\rm R}^2 + (\eta_1 a\Lambda^2)^2}, \tag{4.43}$$

where the η_1 term parameterizes the mass independent O(a) uncertainties in the value of the untwisted quark mass $m_{\rm q}$ (see eqs. 4.22 and 4.25). Expanding in powers of a we have

$$M_{\rm R} \simeq \mu_{\rm R}\Big[1 + \frac{\eta_1 a^2\Lambda^4}{2\mu_{\rm R}^2} + O(a^4)\Big]. \tag{4.44}$$

We observe immediately that if numerically $\mu_{\rm R} < a\Lambda^2$, even if parametrically O(a) terms are absent in (4.44), there is a term of O(a^2) with a coefficient that tends to diverge as soon as $\mu_{\rm R}$ is made smaller and smaller. From this example we can conclude that to have an effective automatic O(a) improvement, without big O(a^2) effects, with a generic choice of the critical mass, such that the uncertainties in the

untwisted quark mass are of order $a\Lambda^2$, we need to have the constraint

$$\mu_{\rm R} > a\Lambda^2. \tag{4.45}$$

From a practical point a view this constraint can be very strong. If we take the reasonable value $\Lambda = 300$ MeV and a lattice spacing $a = 0.1$ fm then the minimal quark mass that can be simulated without being affected by large $\mathrm{O}(a^2)$ effects is $\mu_{\rm R} = 45$ MeV corresponding, in the pseudoscalar sector, roughly to the mass of a kaon made up by two degenerate quarks. It is then clear that in order to go closer to the physical point corresponding to the *up* and *down* quark masses the constraint has to be weakened. From the example of the pole mass (4.44) we immediately understand that the crucial issue is the determination of the critical line and the understanding of its $\mathrm{O}(a)$ uncertainties.

4.3 The critical mass

In this section, to let the interested reader have a general background, we give the basic information on the two main theoretical frameworks used in the discussion on the determination of the critical mass: Symanzik expansion and Wilson chiral perturbation theory (WχPT). We then list the main results and discuss them, omitting some of the technical details of their derivations.

The issue of the choice of the critical line was raised by the work of Aoki and Bär [55] and by the numerical results obtained in [63]. This problem has been further analyzed in several aspects in [56, 57, 64].

We have seen that to obtain automatic $\mathrm{O}(a)$ improvement the untwisted quark mass has to be set to its critical value, i.e. to a value such that in the continuum limit $m_{\rm R} = 0$. To understand how to impose this, it is enough to understand which are the symmetries that are recovered in the continuum if $m_{\rm R} = 0$ and to impose suitable identities on the lattice.

The symmetries are the twisted parity defined in eq. (4.41) and twisted vector symmetry in the isospin direction 1 and 2 (2.42). One way to impose the restoration of twisted vector symmetry is using the PCAC relation, i.e. determining the critical mass setting the PCAC quark mass to zero. To restore twisted parity it is enough to use a twisted parity violating matrix element like a correlator between charged axial and pseudoscalar currents, and setting it to zero. We remark at this point that actually imposing the restoration of twisted parity automatically restores the twisted vector symmetry and vice versa. This can be understood observing that the discrete version of twisted vector symmetry (4.35) times twisted parity (4.41) is a symmetry of the lattice action, i.e. $\mathcal{P}_F^{1,2}$ (2.38).

All these options have been investigated both analytically and numerically. There are two possible approaches to show that the restoration of twisted parity or twisted vector symmetry is enough to ensure automatic O(a) improvement down to quark masses satisfying a weaker constraint than eq. (4.45). One is the analysis, using the Symanzik expansion, of the O(a) effects in the correlators used to define the critical mass. The second one is the use of a suitable modified chiral expansion in order to include discretization errors in the effective Lagrangian describing pion interactions.

4.3.1 Symanzik expansion

One possible way to restore twisted vector symmetry is to tune the bare untwisted quark mass m_0 to a critical value $m_{\rm cr}$ such that the PCAC mass

$$m_{\rm PCAC} = \frac{\sum_{\mathbf{x}} \langle \partial_0 A_0^a(x) P^a(0) \rangle}{2 \sum_{\mathbf{x}} \langle P^a(x) P^a(0) \rangle} \qquad a = 1, 2. \tag{4.46}$$

vanishes for large euclidean times.

It is possible to show that the cutoff effects of the PCAC mass in infinite volume can be schematically written as

$$\eta_1 a \Lambda_{\rm QCD}^2 + \eta_2 a \mu_{\rm R}^2 + \eta_3 a \Lambda \mu_{\rm R}. \tag{4.47}$$

We are here implicitly assuming that the only physical scales of the theory are $\Lambda_{\rm QCD}$ and $\mu_{\rm R}$, i.e. we have already a rough estimate of the critical mass such that $m_{\rm R}$ =O($a\Lambda_{\rm QCD}$). Practically at this point one has several possibilities. For example [65, 66] for each value of $\mu_{\rm q}$ it is possible to determine the critical mass $m_0 = m_{\rm cr}(\mu_{\rm q})$ (see left panel of fig. 2) tuning the PCAC mass to zero, and then to extrapolate the obtained set of $m_{\rm cr}(\mu_{\rm q})$ to $\mu_{\rm q} = 0$ (see right panel of fig. 2). This extrapolated value of $m_{\rm cr}$ (or equivalently $\kappa_{\rm c}$) can then be used to perform simulations for all the values of $\mu_{\rm q}$. In fact from eq. (4.47) we observe that the critical mass has been tuned such that for all the values of $\mu_{\rm q}$ the PCAC mass has at most O($a\mu_{\rm q}$). The slope of the curve in the right plot of fig. 2 is proportional, as it has been discussed in [57, 64, 67], to O(a) cutoff effects related to the discretization errors of the PCAC mass. In other words this slope is proportional to the η_3 term in eq. (4.47). We remind that it is not surprising that the PCAC mass is not automatically O(a) improved since it is an odd quantity under the twisted parity transformations (4.41) and discrete symmetry (4.35).

Another possibility would be after the determination of the function $m_{\rm cr}(\mu_{\rm q})$ to use a different value of $m_{\rm cr}$ such that $m_{\rm PCAC}$ vanishes for each value of $\mu_{\rm q}$ [11].

[11] In practice one could smoothly interpolate the curve $m_{\rm cr}(\mu_{\rm q})$ at the desired value of the twisted mass

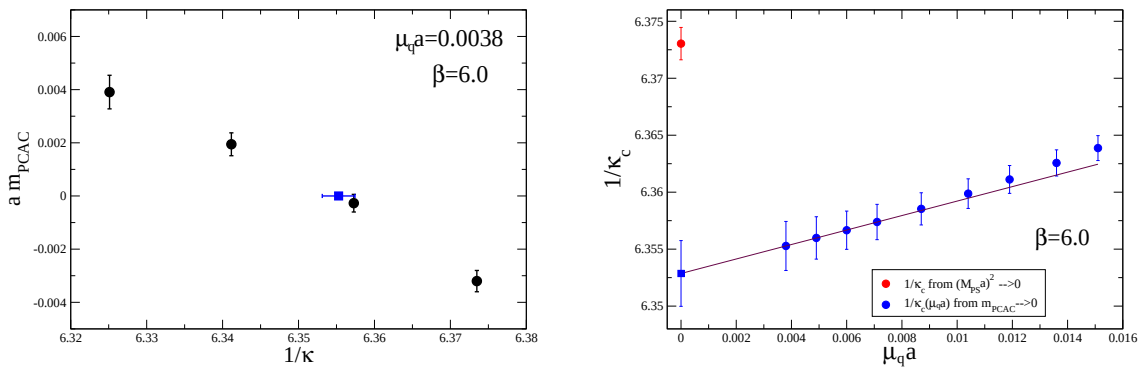


Fig. 2. Determination of the critical mass $m_{\rm c}$ ($\kappa^{-1} = 2am_0 + 8$) for a given value of $\mu_{\rm q}$ at $a = 0.093$ fm (left plot), and extrapolation to $\mu_{\rm q} = 0$ (right plot). The red point in the right plot is the critical mass determined using the "Wilson pion" definition (see sect. 4.3.2 and 4.4 for details).

This procedure has been used in [68] but using a slightly different correlator. One possible way to impose twisted parity restoration, is to tune m_0 to a critical value $m_{\rm cr}$ such that the twisted parity violating correlator

$$a^3 \sum_{\mathbf{x}} \langle A_0^1(\mathbf{x}, x_0) P^1(0) \rangle \tag{4.48}$$

vanishes for large euclidean times x_0. The Symanzik expansion of the correlator (4.48) is, in form, identical to the one of the PCAC mass (4.47). So the same considerations done for the PCAC mass apply here. In particular if one performs an extrapolation of $m_{\rm cr}(\mu_{\rm q})$ to $\mu_{\rm q} = 0$, the cutoff effects of the critical mass would be at most of $\mathrm{O}(a\mu_{\rm q})$, while if $m_{\rm cr}$ is tuned to have twisted parity restoration for each value of $\mu_{\rm q}$ then the critical mass is tuned such that $m_{\rm PCAC} = 0$ for each lattice spacing and each twisted mass value.

Another possible way to fix the critical mass, especially practical for expensive dynamical simulations, is to compute the critical mass, using the PCAC relation at the smallest value of $\mu_{\rm q} = \mu_{\rm min}$, and then use this critical mass for all the simulation points at heavier twisted masses. This method has been used in a recent work [69] where for the first time large scale dynamical simulations have been performed with Wtm. This is justified if at different lattice spacings the values of $\mu_{\rm R}$ where $m_{\rm cr}$ is computed are properly matched. Using again eq. (4.47) one sees that for all the values of $\mu_{\rm q} > \mu_{\rm min}$ the PCAC mass has cutoff effects at most of $\mathrm{O}(a\mu_{\rm min})$.

We immediately observe that all these methods tune the critical mass such that the PCAC mass is identically zero or at most an $\mathrm{O}(a\mu_{\rm q})$.

To obtain the same result it is possible to use a clover term in the action with a

non-perturbatively tuned value for $c_{\rm sw}$. This will remove by definition the $O(a\Lambda)$ in the PCAC mass, leaving again the PCAC mass with $O(a\mu_{\rm q})$. The critical mass can be determined also in the standard Wilson framework, with $\mu_{\rm q} = 0$. In this case a non-perturbatively tuned value for $c_{\rm sw}$, will again eliminate the $O(a\Lambda)$ errors, leaving only $O(am_{\rm q})$ cutoff effects in the PCAC mass. Performing then a chiral extrapolation at fixed lattice spacing would implicitly determine the critical mass $m_{\rm cr}$ up to $O(a^2)$. The only disadvantage of using this method with $\mu_{\rm q} = 0$ being that for quenched computations a long extrapolation to the chiral point is needed because of the occurrence of exceptional configurations.

The same considerations apply if the critical mass is determined in large volume simulations using Schrödinger Functional boundary conditions. If the standard Schrödinger Functional is used in a small volume ($L \lesssim 0.5$ fm), the PCAC mass properly improved (computed with the proper values of $c_{\rm sw}$, $c_{\rm A}$) can be used to determine the critical mass with residual discretization errors of $O(a^2)$ [43] without almost any extrapolation to the chiral limit. This is possible because the standard chirally breaking boundary conditions protect the spectrum of the Wilson operator from the appearence of very small eigenvalues, allowing simulations almost at the chiral point.

What is relevant is that the cancellation of the $O(a\Lambda)$ obtained with a properly tuned $c_{\rm sw}$ is mass independent. This allows a tuning to full twist without a recomputation of the critical mass. In fact in refs. [70–72] old determinations [12] [43, 73, 74] of the critical mass with clover improved fermions have been used.

To summarize, all the determinations of the critical mass based on correlators which violate twisted parity and twisted vector symmetry, are such that the PCAC mass is affected at most by $O(a\mu_{\rm q})$ cutoff effects.

If we recall the example of the polar mass (4.44) we see that now we could relax the constraint (4.45). It is possible to show [57] that this observation is actually true in general.

In [57], it has been shown that the cutoff effects which diverge at small quark masses previously discussed (see eq. 4.44), so called infrared divergent (IR) cutoff effects, are a general property of Wtm. In general a Wtm correlator will be automatically $O(a)$ improved at full twist, but could suffer from numerically large $O(a^2)$ effects as soon as $\mu_{\rm R} \simeq a\Lambda^2$. The result of ref. [57] can be summarized as follows: in the Symanzik expansion of the lattice correlator $\langle\Phi\rangle$ defined in eq. (4.7) at order a^{2k}

[12] In [70] $m_{\rm cr}$ has been recomputed only at one lattice spacing.

($k \geq 1$) there are terms of the kind

$$\left(\frac{a}{M_\pi^2}\right)^{2k}, \qquad k \geq 1 \tag{4.49}$$

proportional to the matrix element

$$|\langle\Omega|\mathcal{L}_1|\pi^0(\mathbf{0})\rangle_0|^{2k}. \tag{4.50}$$

It is possible to recognize the $(a/\mu_{\rm R})^2$ of eq. (4.44) as the $k = 1$ case in eq. (4.49) recalling that to a first approximation $M_\pi^2 \propto \mu_{\rm R}$. The terms in eq. (4.49) are called leading infrared divergent cutoff effects, and they come from continuum correlators where $\mathcal{L}_1$ is inserted $2k$ times. In the following, unless specified, we use the same notation for the dimension 5 fields and the corresponding operators. A bit of notation is needed now: this is the continuum (see the index 0) matrix elements of the dimension 5 Lagrangian that appears in the Symanzik expansion of a lattice correlator defined by

$$\mathcal{L}_1 = c_0\mathcal{O}_0 + c_1\mathcal{O}_1 + c_5\mathcal{O}_5 \tag{4.51}$$

where $\mathcal{O}_{0,1}$ are defined in eq. (4.32) and $\mathcal{O}_5$ in eq. (4.39). Actually being proportional to $\mu_{\rm q}^2$ the field $\mathcal{O}_5$ is not relevant for the following discussion. We also remind that we work at full twist with an unspecified estimate of the critical mass $m_{\rm cr}$.The dimension 5 Lagrangian $\mathcal{L}_1$ has the quantum numbers of a neutral pion field because we recall we are in the twisted basis at full twist. Then it has a non-zero matrix element between the vacuum $\langle\Omega|$ and the neutral pion at rest $|\pi^0(\mathbf{0})\rangle$ states.

To remove these dangerous cutoff effects, in ref. [57] it is proven that, setting the critical mass imposing the restoration of the twisted vector symmetry, the leading infrared divergent cutoff effects are removed. In particular in [57] it is suggested to compute for each value of $\mu_{\rm q}$ the critical mass imposing that the correlator in eq. (4.48) vanishes for large euclidean times, and then to extrapolate to $\mu_{\rm q} = 0$. This leads to the result

$$\lim_{\mu_{\rm q}\to 0} |\langle\Omega|\mathcal{L}_1|\pi^0(\mathbf{0})\rangle_0|^{2k} = 0. \tag{4.52}$$

Incidentally in the same paper it is also suggested that an alternative possibility would be to use non-perturbatively improved clover fermions which would set the operator $\mathcal{O}_1$ to zero. The conclusion of ref. [57] is that with an "optimal" choice of the critical mass, obtained as just discussed, Wtm is automatically O(a) improved for

$$\mu_{\rm R} > a^2\Lambda^3. \tag{4.53}$$

Before ending the section we want to briefly show with an example how even without an extrapolation to $\mu_{\rm q} = 0$ the method of ref. [69] does not imply the existence of infrared divergent cutoff effects.

We set the PCAC mass to zero at a value $\mu_{\rm R} = \mu_1$ and as an example we consider again the polar mass (4.43) up to $\mathrm{O}(a^2)$ at a value $\mu_{\rm R} = \mu_2 \neq \mu_1$

$$M_{\rm R} \simeq \mu_R \left[1 + \frac{1}{2}\eta_2^2 a^2 \mu_2^2 \left(1 - \frac{\mu_1^2}{\mu_2^2}\right)^2 + \right.$$
$$\left. + \frac{1}{2}\eta_3^2 a^2 \Lambda^2 \left(1 - \frac{\mu_1}{\mu_2}\right)^2 + \eta_2\eta_3 a^2 \Lambda \left(\mu_2 + \mu_1\right) \left(1 - \frac{\mu_1}{\mu_2}\right)^2 \right] . \qquad (4.54)$$

It is then clear from this example that no dangerous infrared cutoff effects appear if $\mu_2 > \mu_1$. Even if $\mu_2 \lesssim \mu_1$ no big enhancement are visible and if $\mu_2 \gg \mu_1$ the cutoff effects take the standard form as the PCAC mass would have been set to vanish at $\mu_{\rm q} = 0$.

All the methods we have discussed before show that all the determinations of the critical mass imply at most $\mathrm{O}(a\mu_{rmq})$ cutoff effects in the PCAC mass. We will see in the next section that actually from a purely theoretical point of view, all the determinations of the critical mass will have this property. While certainly the analysis of ref. [57] is correct, if we consider only $\mathrm{O}(a)$ cutoff effects there is really no "optimal" choice of the critical mass, but they are all equivalent. We will analyze further this point, in particular because from a practical point of view this might not be the case.

4.3.2 Wilson chiral perturbation theory

An alternative method to analyse cutoff effects in physical observables at low energies is to apply the methods of chiral perturbation theory to the Wtm action, i.e. at non-zero lattice spacing. The discretization errors can be included systematically in a combined expansion in the lattice spacing and in the quark mass.

We recall first the basic principles of chiral perturbation theory (χPT) in the continuum considering $N_f = 2$ flavour QCD. If the quark masses are set to zero the QCD action (2.1) is symmetric under the chiral group $SU_{\rm L}(2) \times SU_{\rm R}(2)$. One then *assumes* that the theory spontaneously breaks this symmetry (see ref. [75] and refs. therein) down to $SU_{\rm V}(2)$ [13] . The symmetry manifests itself in the occurrence of $2^2 - 1 = 3$ pseudoscalar Goldstone bosons. In reality the QCD action contains a mass term which breaks the symmetry and this appears in the non-conservation of the Nöther currents (2.18,2.19). Since the masses of the u and d quarks are small, the low energy

[13] Strictly speaking for $N_f = 2$, chiral symmetry is spontaneously broken when $(m_u + m_d) \to 0$. In the following we will concentrate on degenerate light quarks and neglect physical isospin breaking effects.

properties associated with chiral symmetry should show a small deviation due to the quark masses. A rough estimate of the size of these deviations should be given by the ratio between the quark masses and the intrinsic QCD scale, giving a violation of a few percent.

The low energy structure of the correlation functions in QCD depends on the size of the quark masses. Heavy quarks play a minor role because their degrees of freedom are frozen at low energies. Here we consider only two flavours u and d. This is suitable for our purposes where we consider a lattice action for two degenerate flavours. In this restricted framework we are able to discuss only the dependence of the correlation functions on the u and d quark masses, and the remaining quark masses are fixed. The method we are going to briefly review [13, 76] is the extension of the analysis carried by Weinberg [77] for the S-matrix elements, to an expansion of correlation functions in powers of the momenta and the quark masses.

The method consists in adding space dependent external fields to the QCD Lagrangian which transform accordingly in order to keep the Lagrangian invariant under a local chiral transformation. Then using the assumption of spontaneous symmetry breaking, it is possible to write a general low energy effective chiral Lagrangian where the pion fields, i.e. the fields corresponding to the Goldstone bosons, are collected in a unitary matrix that automatically fulfills the requirements of chiral symmetry. The source terms of the QCD Lagrangian are collected in the effective Lagrangian according to their symmetry transformations under chiral symmetry. The behaviour at small momenta and quark masses of the QCD correlation functions can be recovered *matching* them with the expansion of the chiral effective Lagrangian in powers of the derivative of the external fields and the fields themselves. We remark that this low-energy expansion is not a Taylor series: the pions generate poles at small momenta. The correlation functions admit a Taylor expansion only if the momenta are much smaller then the pion mass. So the power counting will be identified by the pion momentum p^2 and the pion mass M_π^2 (or the quark mass). In particular they will be treated to be both small but with the value of the ratio p^2/M_π^2 fixed and unconstrained.

The QCD Lagrangian with external fields reads

$$\mathcal{L} = \mathcal{L}_0 + \overline{\chi}(x)\Big[s(x) + i\gamma_5 p(x)\Big]\chi(x). \tag{4.55}$$

For simplicity, since not needed in the following analysis, we neglect vector and axial external fields and θ-terms induced by the anomaly. $\mathcal{L}_0$ is the massless QCD Lagrangian that includes the gauge part,[14] and the external fields $s(x)$ and $p(x)$

[14] It could in principle also include the heavier quarks.

are 2×2 Hermitean matrices in flavour space (we assume that $p(x)$ is traceless)

$$s(x) = s^0(x)\mathbb{I} + s^a(x)\tau^a, \qquad p(x) = p^a(x)\tau^a. \tag{4.56}$$

The connected correlation functions are obtained performing functional derivatives with respect to the sources $s(x)$ and $p(x)$ on the generating functional defined as

$$\mathcal{W}[s,p] = \log \mathcal{Z}[s,p], \qquad \mathcal{Z}[s,p] = \int D[\overline{\chi},\chi]D[U]\, \mathrm{e}^{-S[s,p]}, \qquad S[s,p] = \int d^4x \mathcal{L}, \tag{4.57}$$

and then fixing them at their physical value: in the twisted basis the correlation functions for massive quarks at full twist are obtained expanding around $s = 0$ and $p = \mu_\mathrm{q}\tau^3$. For example

$$\langle P^a(x)P^b(y)\rangle = \left(\frac{-i}{2}\frac{\delta}{\delta p^a(x)}\right)\left(\frac{-i}{2}\frac{\delta}{\delta p^b(y)}\right)\mathcal{W}[s,p]\Big|_{s=0,p=\mu_\mathrm{q}\tau^3}. \tag{4.58}$$

The local $SU_\mathrm{L}(2) \times SU_\mathrm{R}(2)$ transformation of the fields is

$$\chi(x) \to V_R(x)\frac{1}{2}(1+\gamma_5)\chi(x) + V_L(x)\frac{1}{2}(1-\gamma_5)\chi(x) \tag{4.59}$$

$$s(x) + ip(x) \to V_R(s(x) + ip(x))V_L^\dagger. \tag{4.60}$$

On the other side, the pion fields are collected in a unitary matrix Σ which transforms according to the linear representation

$$\Sigma(x) \to V_R\Sigma(x)V_L^\dagger. \tag{4.61}$$

The singlet field is eliminated imposing $\det\Sigma = 1$, where det is applied in flavour space.

The effective chiral Lagrangian will be a function of the pion fields and their derivatives together with the external fields

$$\mathcal{L}_\chi = \mathcal{L}_\chi(\Sigma, \partial_\mu\Sigma, s, p, ...). \tag{4.62}$$

The order of the arguments reflects their low-energy dimensions: Σ counts as a field of order 1, $\partial_\mu\Sigma$ as order p and $s(x)$,$p(x)$ as order p^2. The general effective Lagrangian of order 1 is only a function of Σ and since it has to be chiral invariant it can only depend on $\det\Sigma$ or $\mathrm{Tr}\left[\left(\Sigma\Sigma^\dagger\right)^n\right]$ where Tr is applied in flavour space, i.e. an irrelevant constant. We conclude that chiral symmetry implies a leading derivative coupling. The matrix Σ that collects the pion fields can be written as

$$\Sigma(x) = \Sigma_0 \exp\left(i\frac{\pi^a(x)\tau^a}{f^2}\right) \tag{4.63}$$

where $\pi^a(x)$ are the pion fields, the dimensionfull constant f is the decay constant in the chiral limit normalized to $f_\pi = 93$ MeV, and Σ_0 is the vacuum expectation value of Σ, that breaks the chiral symmetry down to $SU_{\rm V}(2)$. The pion fields parametrize the fluctuations around Σ_0.

The most general form for the effective Lagrangian consistent with chiral symmetry is given by

$$\mathcal{L}_\chi^{(2)} = \frac{f^2}{4}\Big[\langle\partial_\mu\Sigma(x)^\dagger\partial_\mu\Sigma(x)\rangle + \langle\sigma(x)\Sigma(x)^\dagger + \sigma(x)^\dagger\Sigma(x)\rangle\Big], \tag{4.64}$$

where the brackets $\langle\cdot\rangle$ here indicate the trace in flavour space. The field $\sigma(x)$ collects the external field dependence of the effective Lagrangian according to chiral symmetry

$$\sigma(x) = 2B_0\Big[s(x) + ip(x)\Big]. \tag{4.65}$$

Analogously to what we have done for the quark Lagrangian (4.55) we can do here for the effective chiral Lagrangian, defining the generating functional for connected correlation functions. The strategy is then to equate the correlation functions obtained in the two theories. This will express the QCD correlators as a function of the quark masses and the low energy constants (LEC) f and B_0. Since we are expanding around massless QCD the only scale that can appear is $\Lambda_{\rm QCD}$, so one expects $f \sim B_0 \sim \Lambda_{\rm QCD}$.

To include the discretization errors in effective chiral theory one proceeds in two steps [78]. First, one determines the continuum Symanzik action describing the interactions of quarks and gluons with momenta much smaller than π/a. Discretization errors enter with explicit factors of a, and are controlled by the symmetries (or lack thereof) of the underlying lattice theory. Second, one uses standard techniques to develop a generalized chiral expansion for the Symanzik effective theory. We will call generically this expansion Wilson chiral perturbation theory (WχPT) having in mind a general form for the mass term that includes also the twisted mass case.

The form of the Symanzik effective Lagrangian including the external sources is given by

$$\mathcal{L}_{\rm eff} = \mathcal{L} + a\mathcal{L}_1 + \dots \tag{4.66}$$

with $\mathcal{L}$ given by eq. (4.55) and $\mathcal{L}_1$ by eq. (4.11). In order to ease the construction of the chiral Lagrangian in the following we keep all the terms in $\mathcal{L}_1$ without using the freedom to eliminate them through a redefinition at O(a) of the bare parameters.

At this point it is useful to anticipate the power counting scheme including the lattice spacing a. This is

$$1 \gg m_{\rm R}, \mu_{\rm R}, p^2, a \gg m_{\rm R}^2, \mu_{\rm R}^2, p^4, a^2, m_{\rm R}\mu_{\rm R}, m_{\rm R}p^2, am_{\rm R}, \mu_{\rm R}p^2, a\mu_{\rm R}, ap^2 \gg \dots \tag{4.67}$$

The factors of Λ (with Λ a scale of order $\Lambda_{\rm QCD}$) necessary to make all these quantities dimensionless are implicit from now on unless specified.

We recall that this approach to the description of the lattice data does not require a continuum extrapolation, hence the power counting scheme does not imply that $\mu_{\rm R}$ goes to zero in the continuum limit but represents only an order of magnitude equality. In other words the following formulæ are useful in describing at fixed lattice spacing the quark mass dependence of a given lattice correlator only in a region of quark masses appropriate given the power counting scheme and the value of the lattice spacing.

The next step is to *match* the continuum effective Lagrangian (4.66) into a generalized chiral Lagrangian. At LO the sole term that survives in $\mathcal{L}_1$ is the clover term ($\mathcal{O}_1$ in eq. 4.32), all the other terms being at least of NLO. The key property that allows this matching was noticed by Sharpe and Singleton in ref. [78] where they realized that the *clover term transforms under chiral symmetry exactly as the mass term*. It is the possible to add to the chiral Lagrangian (4.64) a simple source term in order to include the leading discretization effects. Namely the modified LO continuum chiral Lagrangian reads

$$\mathcal{L}^{(2)}_{W\chi} = \frac{f^2}{4}\Big[\langle\partial_\mu\Sigma(x)^\dagger\partial_\mu\Sigma(x)\rangle + \langle\sigma(x)\Sigma(x)^\dagger + \sigma(x)^\dagger\Sigma(x)\rangle + \langle A(x)\Sigma(x)^\dagger + A(x)^\dagger\Sigma(x)\rangle\Big]. \tag{4.68}$$

At the end of the analysis the sources are set to their physical value

$$\sigma(x) \to 2B_0(m_{\rm R} + i\tau^3\mu_{\rm R}), \qquad A(x) \to 2W_0 a \tag{4.69}$$

where W_0 is an unknown dimensionful constant which parametrizes the leading cutoff effects. We remark that if the $c_{\rm SW}$ coefficient would be set to its "correct" non-perturbative value we would have $W_0 = 0$. This does not mean that all the $\mathrm{O}(a)$ terms will disappear, because there will be $\mathrm{O}(a)$ terms at NLO, that would have to be cancelled by other improvement coefficients.

Because of the chiral transformation properties of the clover term, the LO Lagrangian (4.68) is unchanged from its continuum form if one shifts the external sources

$$\sigma' \equiv \sigma + A. \tag{4.70}$$

This at the quark level corresponds to a redefinition of the untwisted quark mass

$$m_{\rm R} \to m_{\rm R} + aW_0/B_0 \equiv m'. \tag{4.71}$$

Recalling the definition of $m_{\rm R}$ in eq. (4.22), this is equivalent to a shift in the critical mass. This observation is rather important because it means that at LO all the $\mathrm{O}(a)$ effects in spectral quantities can be reabsorbed in the definition of the quark mass through the offset, or shift, aW_0/B_0. This shift is not measurable, however, since $m_{\rm cr}$

is not known *a priori*. It must be determined non-perturbatively from the simulation itself. The traditional definition is that $m_{\rm cr}$ is the bare mass at which $M_\pi^2 \to 0$ on the Wilson axis, i.e. $\mu_{\rm q} = 0$. Since at LO the chiral Lagrangian (4.68) predicts $M_\pi^2 \propto m'$, we discover that this "Wilson pion" definition of $m_{\rm cr}$ *automatically* includes the shift in critical mass, and chooses the untwisted quark mass to be m'. This remark is important because firstly it tells us that with the standard numerical definition of $m_{\rm cr}$, the pion and vacuum sectors are automatically $O(a)$ improved at LO in WχPT *for any twist angle*, and secondly it indicates that from a theoretical point of view, at least at LO, there is no difference in the critical line computed in this way or by using other methods which set $m' = 0$. We will come back later to this point when analysing numerical results.

Analogously to what we have done in the continuum, we define a polar mass and a twist angle that includes this O(a) shift

$$M' \mathrm{e}^{i\omega'\tau^3} \equiv (m' + i\mu_{\rm R}\tau^3). \tag{4.72}$$

In the continuum the PCAC quark mass (2.18) is the untwisted quark mass which appears in the Lagrangian. If we consider now the lattice PCAC quark mass defined in (4.46), evaluating the correlators at large distances in order to let the single pion state dominate one finds

$$m_{\rm PCAC} = m'. \tag{4.73}$$

This shows that this quantity automatically includes the O(a) offset in the untwisted mass, exactly as the pion definition does. We remark that at this order it does not matter if the critical line is computed on the Wilson axis or with $\mu_{\rm q} \neq 0$.

At NLO we should add to the Symanzik expansion the O(a^2) terms (see eq. 4.67). These can be collected in three categories. First, those that are invariant under Euclidean and chiral symmetries, and they simply modify, in the chiral Lagrangian, the leading order continuum results by a^2, i.e. they lead to an $O(a^2)$ correction to the LEC f [79]. Second, there are four-fermion operators which violate chiral symmetry. In the chiral Lagrangian the corresponding operator is already present, having been produced by two insertions of the clover term [80]. This shows that what is relevant for matching are the symmetries broken by the operators (here, chiral symmetry), and not their detailed form. The four-fermion operators simply change the unknown low energy constant corresponding to a double insertion of the clover term. This also means that using a non-perturbatively $O(a)$ improved quark action, this low energy constant does not vanish. Finally, there are the terms violating Euclidean symmetry. These can be decomposed into Euclidean singlet and non-singlet parts, and can be shown to be of higher order [79].

The detailed form of the Wilson chiral Lagrangian at NLO can be found in many papers and reviews (see for example [81] and refs. therein). Here we want to list the

main results [55, 56, 82, 83] and add some considerations.

The charged pion mass squared at NLO reads

$$M_{\pi^\pm}^2 = 2B_0 M' \left[1 + \frac{2B_0 M'}{32\pi^2 f^2} \log(2B_0 M'/\Lambda_\pi^2)\right] + 2aB_0 M' \cos\omega'(2\delta_W - \delta_{\widetilde{W}}) + 2a^2 w' \cos^2\omega'. \tag{4.74}$$

The first term in the r.h.s. is the continuum NLO result [76] while remaining terms show the impact of a finite lattice spacing. In particular δ_W and $\delta_{\widetilde{W}}$ parametrize NLO $\mathrm{O}(a)$ effects of order Λ_{QCD}. The w' term parametrizes NLO $\mathrm{O}(a^2)$ effects of order Λ_{QCD}^2. We have reabsorbed the scale dependence of the chiral logs in the LEC Λ_π, and $2\delta_W - \delta_{\widetilde{W}}$ is scale invariant. Chiral logs do not contain discretization corrections at this order because the LO discretization errors can be absorbed into σ'.

The result (4.74) shows the different possibilities for removing $O(a)$ errors.

- Non-perturbatively $O(a)$ improve the quark action, in which case $2\delta_W - \delta_{\widetilde{W}} = 0$ and the $O(a)$ term vanishes.
- Use "mass averaging" [11] in which one averages over ω' and $\omega' + \pi$ at fixed M'. This flips the sign of both m' and μ_{R}, and thus of $\cos\omega'$, and cancels the $O(a)$ term.
- Work at full twist, $\omega' = \pm\pi/2$. This removes the $O(a)$ term and, in this case though not in general, also the $O(a^2)$ term. This can be traced back to the exact "charged" twisted chiral symmetry (2.41) of the massless Wtm lattice action (2.28).

There are two further features of the result (4.74). The $O(a)$ errors are determined for every twist angle by the combination $2\delta_W - \delta_{\widetilde{W}}$. In particular, on the Wilson axis, this term predicts an asymmetry in the slopes on the two sides of m_c. The asymmetry is defined by [64]

$$\frac{M_\pi^2(m') - M_\pi^2(-m')}{M_\pi^2(m') + M_\pi^2(-m')}, \qquad \text{with } \mu_{\mathrm{R}} \text{ fixed.} \tag{4.75}$$

Neglecting chiral logs and $\mathrm{O}(a^2)$ terms and setting $\mu_{\mathrm{R}} = 0$ in eq. (4.74) the asymmetry is given by

$$a\frac{m'}{|m'|}\left(2\delta_W - \delta_{\widetilde{W}}\right). \tag{4.76}$$

This asymmetry has been previously observed numerically [84], in the course of the initial studies of the properties of Wtm. I show an example of the results in Fig. 3. The observed asymmetry in fig. 3 can be viewed by the difference between the absolute values of the slopes of the two straight lines that leads to a value for the asymmetry ~ 0.3 [64]. This estimate is consistent with the expected size of $(2\delta_W - \delta_{\widetilde{W}}) \sim \Lambda_{\mathrm{QCD}} \simeq 0.3$ GeV considering that $a^{-1} \approx 1$ GeV.

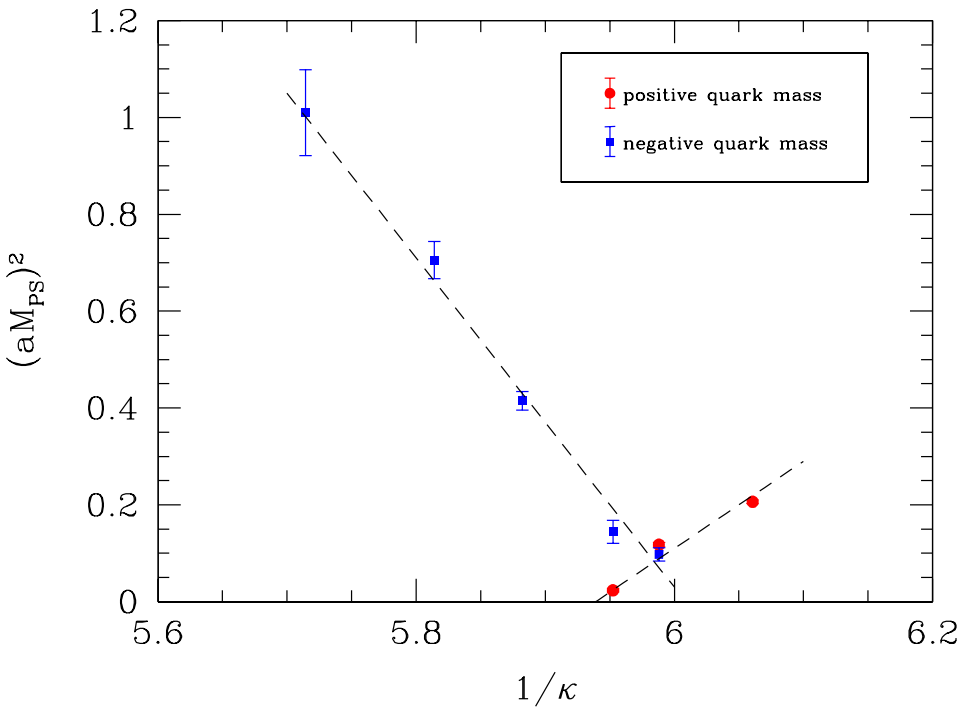


Fig. 3. Unquenched results for $(aM_{\rm PS})^2$ as a function of $\kappa^{-1} = 2m_0 + 8$ for $\mu_{\rm q} = 0$ and with $a \approx 0.2$ fm [84]. Straight lines are to guide the eye.

4.3.3 Full twist

The form of the $O(a)$ correction in the result for M_π^2 in eq. (4.74), is the generic structure of the O(a) terms in all the physical quantities, i.e. all the O(a) cutoff effects are proportional to $a\cos\omega'$. This is the way to observe automatic O(a) improvement in the framework of WχPT. To obtain automatic $O(a)$ improvement one needs $\cos\omega' = O(a)$ and thus $\omega' = \pi/2 + O(a)$. In other words, full twist means at most "up to $O(a)$". I want to briefly explain here in which sense the analysis carried out with the Symanzik expansion and WχPT gives a consistent picture for the determination of the full twist setup.

In sect. 4.2 and 4.3 we have already discussed in the framework of the Symanzik expansion that to achieve automatic O(a) improvement down to masses obeying the constraint (4.53) the untwisted quark mass has to be tuned to be zero up to errors at most of O($a\mu_{\rm q}$). In the power counting scheme (4.67) we assume for the WχPT analysis, with $\mu_{\rm R} \sim a$, an $O(a)$ accuracy in ω' requires $m' = O(a^2)$. This is easily obtained considering that

$$\cos\omega' = \frac{m'}{M'}. \tag{4.77}$$

If we again recall our working power counting it is easy to see that $m' = O(a^2)$ corresponds exactly to the requirement of having a vanishing PCAC quark mass up to $\mathrm{O}(a\mu_\mathrm{q})$ or $\mathrm{O}(a^2)$. So the two analyses are consistent and the result can be summarized as follows: to achieve automatic $\mathrm{O}(a)$ improvement down to a twisted mass which obeys the constraint (4.53) we have to tune the theory to full twist, meaning that the critical mass m_cr has to be tuned such that the PCAC quark mass vanishes up to $\mathrm{O}(a\mu_\mathrm{q})$ or $\mathrm{O}(a^2)$.

The traditional definition of m_cr used with Wilson fermions is to extrapolate m_0 to the point where $M_\pi^2 = 0$. We now consider the NLO expression for the squared charged pion mass (4.74) and set $\mu_\mathrm{q} = 0$. Eq. (4.74) tells us that if one is able to perform a perfect chiral extrapolation including the chiral log, this method is in principle adequate to tune m_cr such that $m' = \mathrm{O}(a^2)$ in the regime $\mu_\mathrm{R} \sim a$.

Alternatively to obtain $m_\mathrm{R} = 0$ in the continuum limit, it is enough to understand which are the symmetries that are recovered in the continuum if $m_\mathrm{R} = 0$ and to impose suitable identities on the lattice. For $m_\mathrm{R} \neq 0$ twisted parity (4.41) and twisted flavour (4.35) are broken symmetries. Enforcing this restoration in particular correlators for $a \neq 0$ gives a non-perturbative determination of the twist angle (or equivalently of m_cr) to full twist.

A way to understand how to impose the restoration of twisted parity symmetry in the continuum limit is to write a correlator which breaks parity in the physical basis. We have seen in sec. 2 which is the relation between fields in the twisted and physical basis. The idea is now to take either (2.12,2.13) or (2.14,2.15) as a *definition* of ω, and enforce parity restoration in a particular correlator. Two examples are the ω_A method [84]

$$\langle \mathcal{V}^2_\mu(x)\mathcal{P}^1(y)\rangle \propto \langle 0|\mathcal{V}^2_\mu|\pi^1\rangle = 0, \tag{4.78}$$

and the ω_P method [56]

$$\langle \mathcal{S}^0(x)\mathcal{A}^3_\mu(y)\rangle \propto \langle 0|\mathcal{S}^0|\pi^3\rangle = 0. \tag{4.79}$$

The correlators are to be evaluated for $x \neq y$ and large euclidean times in order to isolate the single pion contribution. Using (2.12-2.15) one can manipulate these criteria into results for the twist angle in terms of correlators in the twisted basis:

$$\tan\omega_A \equiv \frac{\langle V^2_\mu(x)P^1(y)\rangle}{\langle A^1_\mu(x)P^1(y)\rangle}\,, \quad \tan\omega_P \equiv \frac{i\langle S^0(x)A^3_\mu(y)\rangle}{2\langle P^3(x)A^3_\mu(y)\rangle}\,. \tag{4.80}$$

Full twist occurs when the denominators vanish, i.e

$$\omega_A = \pi/2 \Rightarrow \langle A^1_\mu(x)P^1(y)\rangle = 0\,, \quad \omega_P = \pi/2 \Rightarrow \langle P^3(x)A^3_\mu(y)\rangle = 0\,. \tag{4.81}$$

The correlator in the "ω_P method" includes quark-disconnected contractions and is much more difficult to calculate in practice. The "ω_A method" is used in practice.

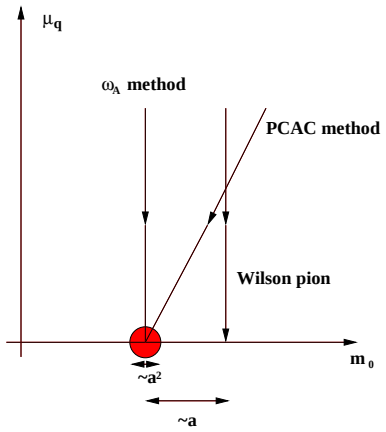


Fig. 4. Sketch of the different methods for working at full twist. The arrows represent the direction one moves to approach the chiral limit (which occurs at $\mu_{\rm q} = 0$). The plot represents the regime in which $M_{\rm R} \sim a$. The regime in which $M_{\rm R} \sim a^2$ is represented by the shaded region. It is discussed in sec. 6. For the "Wilson pion" method the supposed behaviour given the quenched numerical data is plotted. See text for discussion.

One fixes $\mu_{\rm q}$ and varies m_0 until $\omega_A = \pi/2$. The resulting $m_{\rm cr}(\mu_{\rm q})$ depends on the choice of discretization of the axial current (e.g. $O(a)$ improved or not), and, in general, upon the separation $x - y$. In fig. 2 a typical $\mu_{\rm q}$ dependence of the critical line is shown. At large distances, which are used in practice, the pion contribution dominates and the resulting $m_{\rm cr}$ becomes independent of separation. At such distances the "ω_A method" is equivalent to the vanishing of the PCAC mass (4.46). We remind that the determination of ω at full twist does not require any computation of Z-factors [15].

Both methods can be studied in WχPT and at full twist we have [56]:

$$\omega_A = \pi/2 \;\Rightarrow\; \omega' = \pi/2 + a\delta_W\,, \quad \omega_P = \pi/2 \;\Rightarrow\; \omega' = \pi/2\,, \tag{4.82}$$

To summarize: all the known methods to compute the critical line are theoretically equivalent in order to achieve automatic O(a) improvement provided $\mu_{\rm R} > a^2\Lambda^3_{\rm QCD}$. Practically the situation can be very different as we are going to discuss in the next section.

4.3.4 The bending phenomenon: a closed chapter

The discussion up to this point makes clear the importance of accurate tuning to full twist. Initial studies of Wtm in the quenched model observed a phenomenon called "bending". Although this is largely a closed chapter in the history of Wtm, it is worth learning the appropriate lessons. Here we assume that we work in a region of quark masses such that $\mu_{\rm R} \gg a^2$. We will enter into the region where $\mu_{\rm R} \sim a^2$ in sect. 6.

I show in fig. 5, the numerical results for $af_{\rm PS}$ at a fixed value of the lattice spacing ($a = 0.093$ GeV) using several definitions for the critical mass (see the caption for more details). A clear "bending" is observed at smaller quark masses with the "Wilson pion" definition. This bending can be explained taking the LO expression in WχPT for the pseudoscalar decay constant

$$f_{\rm PS} = f \frac{\mu_{\rm R}}{\sqrt{\mu_{\rm R}^2 + m_{\rm PCAC}^2}} \simeq f \left[1 - \frac{1}{2}\left(\frac{m_{\rm PCAC}}{\mu_{\rm R}}\right)^2 + \ ...\right] \ , \tag{4.83}$$

where f is the pion decay constant in the chiral limit and $\mu_{\rm R}$ and $m_{\rm PCAC}$ represent the renormalized twisted and PCAC quark masses respectively. We have already seen that from a theoretical point of view, independently on the definition used for tuning $m_{\rm cr}$, $m_{\rm PCAC}$ vanishes or is a quantity of $O(a\mu_{\rm q})$ or $O(a^2)$. The term $\left(\frac{m_{\rm PCAC}}{\mu_{\rm R}}\right)^2$ causes a deviation of the expected chiral behaviour as soon as $\mu_{\rm R} \simeq m_{\rm PCAC}$. The fact that for the "Wilson pion" definition a "bending" appears for $\mu_{\rm q} \simeq a\Lambda_{\rm QCD}^2$, gives an indirect evidence that $m_{\rm PCAC} = O(a)$. In practice in a quenched simulation, a long extrapolation along the Wilson axis is needed because of the occurrence of exceptional configurations(see sec. 2.9). It is conceivable that performing this long extrapolation without including the chiral logs and in a region of quark masses where the applicability of NLO WχPT is debatable, the critical mass could be determined in such a way that $m_{\rm PCAC}$ is of order a. If this happens, this could generate, as we have seen, large $O(a^2)$ corrections. A possible way to resolve the issue would be to perform chiral fits using NLO WχPT, including $m_{\rm PCAC}$ as a fit parameter for several lattice spacings and then studying the lattice spacing dependence of $m_{\rm PCAC}$.

An alternative approach is to use the clover improved Wtm action (4.18) which removes from the theory all the cutoff effects of the kind $a\Lambda_{\rm QCD}^2$ [57], and to use the equivalent pion and PCAC determination of $m_{\rm cr}$. This is nicely shown in fig. 5 where both the "Wilson-clover pion" definition and the "Wilson-clover PCAC" definition give no evidence of bending down to masses $\mu_{\rm q} \simeq a^2\Lambda_{\rm QCD}^3$ [71].

The final answer is given by a study of the lattice spacing dependence of several physical quantities, with several definitions of $m_{\rm cr}$.

The "Wilson pion" method was used in the first scaling study of Wtm in the quenched model [85]. This study was performed in a region of quark masses where most probably $\mu_{\rm R} \gg a$. Therefore the "Wilson pion" definition was good enough to obtain a clear evidence of automatic $O(a)$ improvement, and no enhanced $O(a^2)$ effects.

In a further publication [66] the PCAC method and the "Wilson pion" method have been compared, obtaining consistent results in the continuum limit but rather different $O(a^2)$ effects. This is clearly seen in the fig. 6 where $f_{\rm PS}r_0$ is plotted as a function of $(a/r_0)^2$ for pseudoscalar masses in the range 297-1032 MeV, obtained

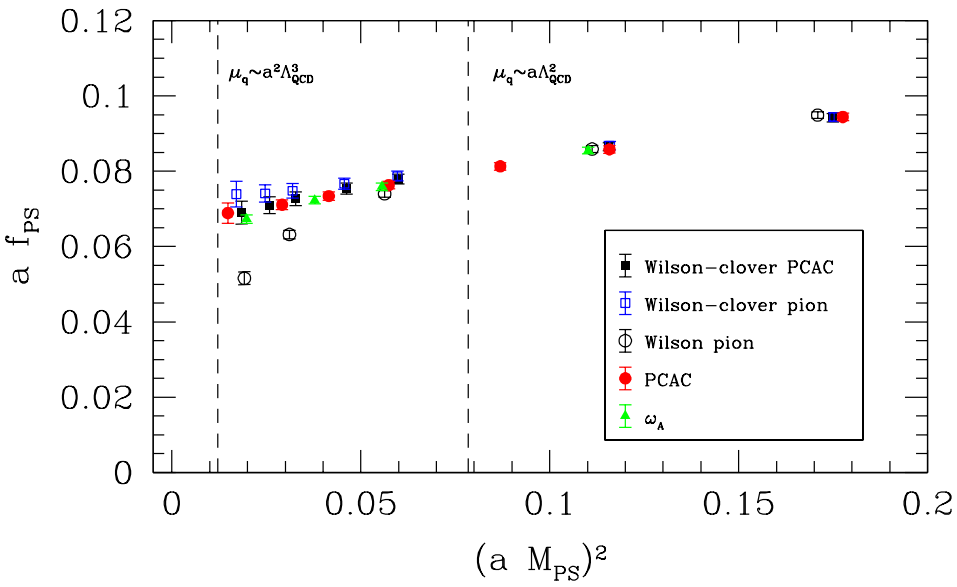
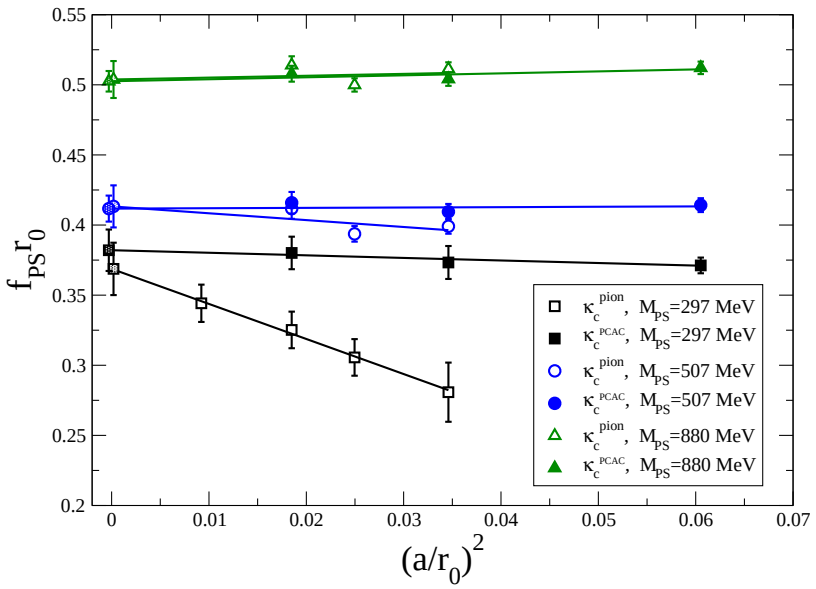


Fig. 5. Chiral behaviour of the pseudoscalar decay constant at fixed lattice spacing $a = 0.093$ fm for several determinations of the critical mass $m_{\rm cr}$: "Wilson-clover PCAC" (■) and "Wilson-clover pion" (□) [71], "Wilson pion" (○) and PCAC (●) [65,66], ω_A (▲) [68].

with both definitions of $m_{\rm c}$. For small enough values of the lattice spacing, the values of $f_{\rm PS} r_0$ show, with both definitions of $m_{\rm cr}$, a linear behaviour in $(a/r_0)^2$. This nicely demonstrates the $O(a)$ improvement for both definitions of the critical mass. However, for the pion definition we notice that the effects of $O(a^2)$ are rather large, in particular at small pseudoscalar meson masses of 297 MeV and 377 MeV. In contrast, the PCAC definition reveals an almost flat behaviour as a function of $(a/r_0)^2$ even at these small pseudoscalar meson masses. In order to take the continuum limit, one should identify the scaling region where the data are well described by corrections linear in $(a/r_0)^2$. This turns out to start at $a = 0.093$ fm with the pion definition of $m_{\rm cr}$ and at $a = 0.123$ fm with the PCAC definition. The values in the continuum limit are obtained separately by performing linear fits to the data in these two regions. The results of these fits are shown in fig. 6 together with the simulation data. It is very reassuring that these independent linear fits lead to completely consistent continuum values.

4.4 The critical mass: summary

All this discussion about the critical mass deserves a summary. In fig. 4 is sketched the approach to the chiral limit according to the different definitions used for the critical mass $m_{\rm cr}$. For the "Wilson pion" definition the supposed behaviour is shown



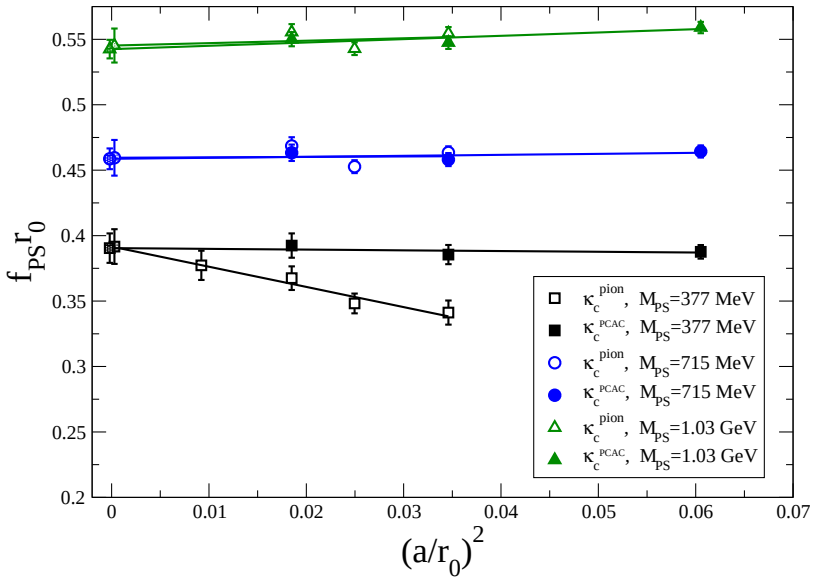


Fig. 6. $r_0 f_{\rm PS}$ as a function of $(a/r_0)^2$ using the "Wilson pion" definition (open symbols) and the PCAC definition (filled symbols) of the critical mass; fits are performed with a linear function in $(a/r_0)^2$ separately for each set.

given by the quenched numerical data. While they are all nominally at full twist: they could show different $O(a^2)$ scaling behaviour depending on the value of the quark mass $\mu_{\rm R}$. In table (4.4) I collect all the definitions discussed and here are

Method	Definition
Wilson pion	$\lim_{m_0 \to m_{\rm cr}} M_\pi^2 = 0$
Wilson-clover pion	$\lim_{m_0 \to m_{\rm cr}} M_\pi^2 = 0$
Wilson-clover PCAC	$\lim_{m_0 \to m_{\rm cr}} m_{\rm PCAC} = 0$
ω_A	$\langle A_\mu^a(x) P^a(y) \rangle = 0 \quad a = 1,2$
ω_P	$\langle A_\mu^3(x) P^3(y) \rangle = 0$
PCAC	$m_{\rm cr} = \lim_{\mu_{\rm q} \to 0} m_{\rm cr}(\mu_{\rm q})$

some considerations:

- "Wilson pion" : this is a valid definition to guarantee automatic O(a) improvement down to $\mu_{\rm R} \sim a$. If this method is used in the quenched case a long chiral extrapolation is needed because of the occurrence of exceptional configurations. The correct extrapolation to the chiral limit, including eventual chiral logs, is crucial in order to have a definition of the critical mass that absorbes the O(a) offset. If the extrapolation is not done correctly this definition can miss the critical line in such a way that $m' = {\rm O}(a)$. This is most probably the reason of the "bending phenomenon".
- "Wilson-clover pion" : this definition has the advantage with respect to the previous one that, if one removes non-perturbatively the O(a) effects in the lattice action, even if the extrapolation is needed it can miss the critical line only by O(a^2). The nice results of ref. [71] indeed seem to indicate that this definition is good enough to avoid the "bending phenomenon". This somehow confirms that the origin of the "bending phenomenon" is the O(a) effects present in the untwisted quark mass.
- "Wilson-clover PCAC" : to this definition the same considerations apply as for the "Wilson-clover pion" method.
- ω_A : this definition (and the equivalent using the PCAC mass), allows a clean determination of the critical line $m_{\rm cr}(\mu_{\rm q})$ for each value of $\mu_{\rm q}$. It can be safely used in the quenched case, because the twisted mass gives a sharp infrared cutoff to the lattice theory. It has the drawback that the unquenched case requires a tuning for each value of $\mu_{\rm q}$ and this could be rather expensive from the computational side.
- ω_P : this definition, theoretically very attractive, has the drawback that it requires the computation of quark disconnected diagrams. These diagrams are usually more difficult to compute so it has mainly an academic interest.
- PCAC : this definition takes the one obtained with the ω_A method (or the equivalent with the PCAC mass) and then extrapolates $m_{\rm cr}(\mu_{\rm q})$ to $\mu_{\rm q} = 0$. The advantage of this definition is that one could perform the extrapolation using a limited range of values of $\mu_{\rm q}$, and then the critical mass mass could be used for all the values of $\mu_{\rm q}$ one is interested in. A possible cheaper, from a computational point of view, alternative has been recently proposed [69] that uses the critical mass

determined at the lowest value of $\mu_{\rm q}$ used in the simulations.

We can conclude this lengthy and technical discussion on the critical mass with the following statement: provided we are away from the region $\mu_{\rm R} \sim a^2\Lambda^3_{\rm QCD}$ all the definitions given above are theoretically equivalent in order to achieve automatic O(a) improvement. The "Wilson pion" definition has to be avoided in the quenched case because the long extrapolation to the chiral limit can induce effective O(a) cutoff effects in the untwisted quark mass.

4.5 Numerical results

The first numerical evidence of automatic O(a) improvement was given in ref. [85], where a first scaling test was performed at a fixed value of the pseudoscalar meson mass around $M_{\rm PS} \simeq 700$ MeV in the quenched model. In this paper, scaling violations of the pseudoscalar decay constant and the vector meson mass have been studied, confirming that, without any improvement coefficient, Wtm at full twist is consistent with automatic O(a) improvement, with first indications that the remaining O(a^2) effects should be small. This very interesting result has triggered a set of quenched studies [63, 65, 66, 68, 86, 87] to further check the property of automatic O(a) improvement [11], and to gain experience with this formulation of lattice QCD. An interesting quantity to compute with Wtm is the pseudoscalar decay con-

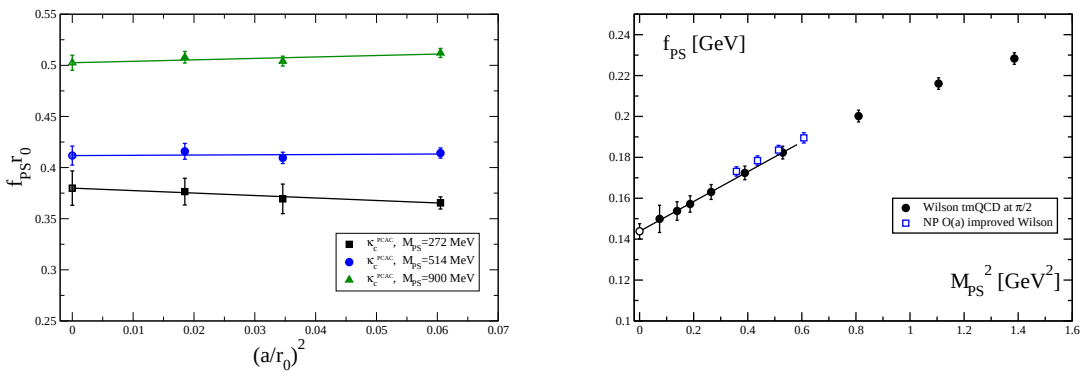


Fig. 7. Left plot: continuum extrapolation of $f_{\rm PS}$ as a function of a^2. Right plot: continuum limit values for $f_{\rm PS}$ as a function of $M^2_{\rm PS}$ in physical units. The empty squares are taken from [54].

stant $f_{\rm PS}$. As it was noted in [53, 85, 88], the computation of $f_{\rm PS}$ does not require any renormalization constant, in contrast of ordinary Wilson fermions, and moreover, given automatic O(a) improvement, does not need the computation of any improvement coefficient. Thus the situation for this quantity is like with Ginsparg-Wilson fermions. The reason for this nice property is that the continuum Ward

identity (2.19), remains exact on the lattice

$$\langle \partial^*_\mu \widetilde{V}^a_\mu(x) O(0)\rangle = -2\mu_{\rm q}\epsilon^{3ab}\langle P^b(x)O(0)\rangle \quad a=1,2, \tag{4.84}$$

(where ∂^*_μ is the lattice backward derivative, and O is a local lattice operator) if one uses a slightly modified point-split vector current

$$\begin{aligned}\widetilde{V}^a_\mu(x) = \frac{1}{2}\Big\{ & \overline{\chi}(x)(\gamma_\mu - 1)\frac{\tau^a}{2}U(x,\mu)\chi(x+a\hat{\mu}) \\ & + \overline{\chi}(x+a\hat{\mu})(\gamma_\mu+1)\frac{\tau^a}{2}U(x,\mu)^{-1}\chi(x)\Big\}.\end{aligned} \tag{4.85}$$

Given the fact that at full twist we have

$$\langle (\mathcal{A}_{\rm R})^1_0(x) P^1(0)\rangle_{(M_{\rm R},0)} = \langle (V_{\rm R})^2_0(x) P^1(0)\rangle_{(m_{\rm R},\mu_{\rm R})}, \tag{4.86}$$

inserting a complete set of states in a standard fashion on the r.h.s. of eq. (4.86) and using the PCVC relation (4.84) we obtain

$$f_{\rm PS} = \frac{2\mu_{\rm q}}{M^2_{\rm PS}}|\langle 0|\hat{P}^a|PS\rangle| \qquad a=1,2 \tag{4.87}$$

where $M_{\rm PS}$ is the charged pseudoscalar mass and $|PS\rangle$ denotes the corresponding pseudoscalar state.

In fig. 7 (left plot) the continuum limit of $r_0 f_{\rm PS}$, the critical mass being computed with the PCAC method, is shown, from ref. [66] as a function of $(a/r_0)^2$. The scaling is consistent with being of $\mathrm{O}(a^2)$, and moreover it is reassuring that the $\mathrm{O}(a^2)$ effects are rather small for all the pseudoscalar masses investigated down to $M_{\rm PS} = 272$ MeV. The right panel of fig. 7 shows the chiral behaviour of the continuum pseudoscalar decay constant [66], compared with the non-perturbatively $\mathrm{O}(a)$ improved data of [54]. We remark that this comparison is purely illustrative since it is in the quenched model, and the simulations with clover fermions had to stop around $M_{\rm PS} \simeq 500$ MeV due to the appearance of exceptional configuration. Using a linear extrapolation of these data to the chiral limit (performed on the six smallest masses) gives the values of the pion and kaon decay constant f_π and f_K (the latter in the $SU(3)$ symmetric limit). The ratio of the two gives $f_K/f_\pi = 1.11(4)$, which is 10% smaller than that obtained experimentally. This is however consistent with what was observed in previous quenched calculations [89].

Another interesting quantity that has been computed is the vector meson mass. Applying the standard axial rotation (2.6) we obtain for $\omega = \frac{\pi}{2}$

$$\langle (\mathcal{V}_{\rm R})^{1,2}_\mu(x)(\mathcal{V}_{\rm R})^{1,2}_\mu(0)\rangle_{(M_{\rm R},0)} = \langle (A_{\rm R})^{2,1}_\mu(x)(A_{\rm R})^{2,1}_\mu(0)\rangle_{(m_{\rm R},\mu_{\rm R})}. \tag{4.88}$$

Another possible interpolating field for the vector channel is given by the following component of the tensor current

$$\mathcal{T}_k^a = \bar{\psi}\sigma_{0k}\frac{\tau^a}{2}\psi. \tag{4.89}$$

This current is invariant under the rotation (2.6), so the vector meson mass can be extracted from the correlators

$$C_A^a(x_0) = \frac{a^3}{3}\sum_{k=1}^{3}\sum_{\mathbf{x}}\langle A_k^a(x)A_k^a(0)\rangle \quad a = 1,2 \tag{4.90}$$

$$C_T^a(x_0) = \frac{a^3}{3}\sum_{k=1}^{3}\sum_{\mathbf{x}}\langle T_k^a(x)T_k^a(0)\rangle \quad a = 1,2 \tag{4.91}$$

One observation [66] is that the tensor correlator systematically shows smaller statistical fluctuations.

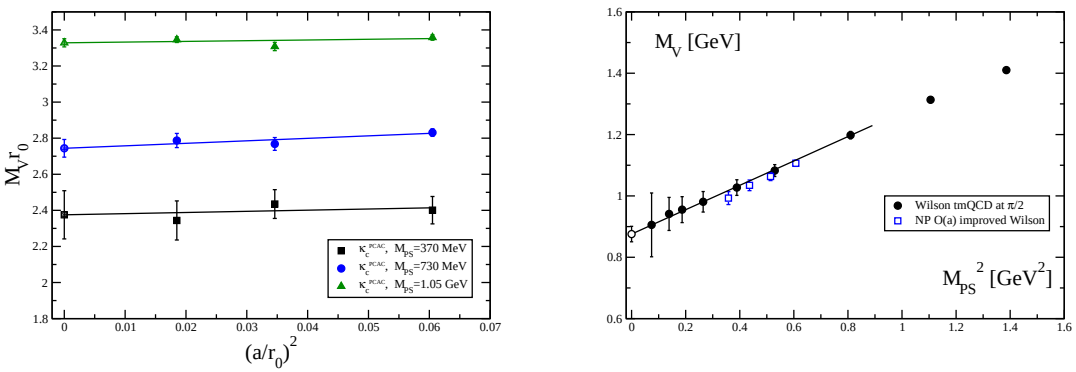


Fig. 8. Left plot: continuum extrapolation of $M_{\rm V} r_0$ as a function of $(a/r_0)^2$. Right plot: continuum limit values of the vector meson mass (filled circles) as a function of the pseudoscalar meson mass squared. The continuum limit vector masses obtained with non-perturbatively improved Wilson fermions (open squares) [54] are also plotted.

In the left plot of fig. 8 we show the results for the vector meson mass as a function of $(a/r_0)^2$. Again, even for small pseudoscalar meson masses, the behaviour of the vector meson mass is almost flat in $(a/r_0)^2$, indicating that $O(a^2)$ lattice artefacts are also small for this quantity. The lines in fig. 8 (left panel) represent linear fits of these data as a function of $(a/r_0)^2$. The continuum extrapolated values for the vector meson mass are presented in the right plot of fig. 8. As a function of the pseudoscalar meson mass squared, they show a linear behaviour. In fig. 8 we also plot the continuum values obtained with non-perturbatively improved Wilson fermions [54]. The results of a linear extrapolation (performed with the seven smallest masses) are used to compute the values of M_ρ and of M_{K^*} (the latter in the $SU(3)$ symmetric limit). As already observed in quenched calculations where the scale is determined through r_0, these values turn out to be $10-15\%$ larger than the experimental values.

Despite the fact that Wtm is a relatively new lattice action, extended scaling tests with mesonic quantities in large volumes have shown beyond any reasonable doubt that automatic $O(a)$ improvement is at work, i.e. at the price of tuning one parameter, namely the critical mass $m_{\rm cr}$, the physical correlation functions exhibits only $O(a^2)$ scaling violations. The issue of the choice of the critical mass can be summarized as follows: provided the definition of the critical mass is theoretically and practically valid each definition leads to automatic $O(a)$ improvement. This statement obviously does not include regions of the bare parameters where phase transitions can occur. In these regions the validity of the Symanzik expansion itself can be questioned. The importance of using both the Symanzik expansion and its application with χPT theory has been shown in all its power. Obviously the remaining $O(a^2)$ contributions of the theory are not predictable, and extensive non-perturbative simulations have to be performed in order to understand the amount of the remaining scaling violations. In the quenched model the remaining $O(a^2)$ scaling violations are very small for a wide range of pseudoscalar masses ($300\text{MeV} \lesssim M_{\rm PS} \lesssim 1\text{GeV}$). Preliminary results [90, 91] indicate that this is true also for $N_f = 2$ dynamical simulations.

5 The physical basis

In the previous two sections we have seen how renormalizability and O(a) cutoff effects of Wtm can be analyzed using the *twisted basis*. In the twisted basis the Wilson term takes the standard form while the mass term takes a "twisted" form. In this section we want to rederive some of the results already presented using the so called *physical basis* [11]. The physical basis is obtained from the twisted basis performing an axial rotation in the τ^3 isospin directionin in the bare lattice theory. If one rotates the bare fields in the action and in the correlation functions, the physics is completely unchanged and correlation functions calculated before and after the rotation are the same on every single gauge configuration. This happens because what matters are the relative angles between the flavour-Dirac directions of the mass term and the Wilson term. These angles are not changed by a bare field rotation.

In the physical basis the Wilson term is chirally rotated while the mass term takes the standard form. The advantage of this basis compared to the twisted one is that the dictionary of the correlation functions is unchanged since after performing the continuum limit, the continuum QCD action takes the standard form. On the other side the dictionary has to be changed from the standard one, in the renormalization process, because the Wilson term is now chirally rotated.

5.1 Chirally rotated Wilson term

The setup is identical to the one described in sect. 2.3. The only difference is the basis in which the fermion action is written, namely in this section the *physical basis* given by the set of fermion fields $\{\psi, \overline{\psi}\}$. For a $SU(2)$ flavour doublet of mass degenerate quarks in the physical basis the action has the form

$$S_{\rm F}[\psi, \overline{\psi}, U] = a^4 \sum_x \overline{\psi}(x) \Big[D_{\rm tW}(\omega) + M \Big] \psi(x), \tag{5.1}$$

where

$$D_{\rm tW}(\omega) = \frac{1}{2}\{\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - ar{\rm e}^{-i\omega\gamma_5\tau^3}\nabla^*_\mu\nabla_\mu\}, \tag{5.2}$$

is the twisted Wilson (tW) operator, ∇_μ, ∇^*_μ are the standard gauge covariant forward and backward covariant derivatives defined in app. A and M is the standard mass term.

To ease the discussion in this section we will concentrate on the full twist case

$\omega = \pi/2$ and we set $r = 1$.Then eq. (5.1) becomes

$$S_{\rm F}[\psi, \overline{\psi}, U] = a^4 \sum_x \overline{\psi}(x) \Big[D_{\rm tW} + M \Big] \psi(x), \tag{5.3}$$

with

$$D_{\rm tW} \equiv D_{\rm tW}(\omega = \pi/2) = \frac{1}{2} \Big[\gamma_\mu (\nabla_\mu + \nabla^*_\mu) + a i \gamma_5 \tau^3 \nabla^*_\mu \nabla_\mu \Big], \tag{5.4}$$

The choices $\omega = \pi/2$ (and equivalently $\omega = -\pi/2$) is particularly useful because as we have seen in sect. 4 it can be shown [11] that, despite the fact that the theory is not fully O(a) improved, cancellation of O(a) effects in quantities of physical interest (like energies and operator matrix elements) is automatic. We will prove again this property in this section using the physical basis.

We shortly recall now the symmetries of the lattice action given in eq. (5.3): gauge invariance, lattice rotations and translations, charge conjugation $\mathcal{C}$ (see app. B for the definition), and the $U(1)$ transformations associated with fermion number. It differs from standard Wilson fermions in two important ways. First, the flavour $SU_{\rm V}(2)$ symmetry is broken explicitly by the Wilson term down to the $U_{\rm V}(1)_3$ subgroup with diagonal generator τ_3

$$U_{\rm V}(1)_3 : \begin{cases} \psi(x) \to \exp(i \frac{\alpha_V}{2} \tau^3) \psi(x), \\ \overline{\psi}(x) \to \overline{\psi}(x) \exp(-i \frac{\alpha_V}{2} \tau^3). \end{cases} \tag{5.5}$$

In sect. 2.4.1 we have seen that Wtm preserves a subgroup of chiral symmetry. In the physical basis this property is even more transparent since the lattice action (5.3) with zero mass ($M = 0$) is invariant under the standard axial transformations

$$U_{\rm A}(1)_{1,2} : \begin{cases} \psi(x) \to \exp(i \frac{\alpha_A}{2} \gamma_5 \tau^{1,2}) \psi(x), \\ \overline{\psi}(x) \to \overline{\psi}(x) \exp(i \frac{\alpha_A}{2} \gamma_5 \tau^{1,2}). \end{cases} \tag{5.6}$$

The massless theory (eq. 5.3 with $M = 0$) is invariant under the group transformations

$$U_{\rm A}(1)_1 \otimes U_{\rm A}(1)_2 \otimes U_{\rm V}(1)_3. \tag{5.7}$$

The "charged" sector has a continuum like behaviour and the exact symmetry (5.7) protects the charged pion from chirally breaking cutoff effects.

The discrete version of this symmetry

$$\mathcal{R}_5^{1,2} : \begin{cases} \psi(x) \to i \gamma_5 \tau^{1,2} \psi(x) \\ \overline{\psi}(x) \to i \overline{\psi}(x) \gamma_5 \tau^{1,2} \end{cases} \tag{5.8}$$

is still a symmetry of the massive lattice action (5.4) if combined with a sign change

of the mass

$$\widetilde{\mathcal{R}}_5^{1,2} \equiv \mathcal{R}_5^{1,2} \times [M \to -M], \tag{5.9}$$

analogously to what happens in continuum QCD.

To understand the structure of the counterterms, we can use the symmetries of the lattice action (5.3) as we have done in the twisted basis. The counterterms to the action with dimension less or equal four are

$$\mathrm{tr}\{F_{\mu\nu}F_{\mu\nu}\}, \quad i\overline{\psi}\gamma_5\tau^3\psi, \quad M\overline{\psi}\psi. \tag{5.10}$$

We notice immediately that quantum corrections imply the necessity to add to the lattice action a counterterm $i\overline{\psi}\gamma_5\tau^3\psi$ with a linearly divergent coefficient. This is not surprising since this is the term that corresponds to the critical mass introduced in sect. 2, which is the linear divergence induced by the presence of the Wilson term.

On the contrary because of the $\widetilde{\mathcal{R}}_5^{1,2}$ symmetry (5.9), the operator $\overline{\psi}\psi$ comes with a coefficient odd in M, and the mass is renormalized only multiplicatively. To state it differently, for zero quark mass the theory still preserves a remnant of chiral symmetry. The residual $U_{\mathrm{V}}(1)_3$ symmetry (5.5) forbids bilinears containing flavour matrices $\tau^{1,2}$. The parity flavour symmetry $\mathcal{P}_F^{1,2}$ defined in eq. (2.38) takes the same form in the two bases and thus is still a symmetry of the lattice action (5.3). This symmetry requires that parity and flavour are violated together so it forbids flavour singlet parity violating terms $\overline{\psi}\gamma_5\psi$ and $\epsilon_{\mu\nu\rho\sigma}F_{\mu\nu}F_{\rho\sigma}$, as well as the flavour violating, parity even, operator $\overline{\psi}\tau_3\psi$. It is easy to check that all the dimension four operators which violate parity or isospin or both are ruled out by $\mathcal{P}_F^{1,2}$. The lattice theory has to be modified in order to include the power divergent subtraction, and to keep consistency between the basis we write the lattice action

$$S_{\mathrm{F}}[\psi,\overline{\psi},U] = a^4 \sum_x \overline{\psi}(x)\left\{\frac{1}{2}\left[\gamma_\mu(\nabla_\mu+\nabla_\mu^*) + i\gamma_5\tau^3\left(a\nabla_\mu^*\nabla_\mu - m_{\mathrm{cr}}\right)\right] + M\right\}\psi(x). \tag{5.11}$$

One can easily check now that this action is completely equivalent from the action in the twisted basis (2.28), just performing the rotations (2.6) with $\omega = \pi/2$ and identifying $m_0 = m_{\mathrm{cr}}$ and $M = \mu_{\mathrm{q}}$. The final continuum theory has now the standard QCD form

$$S_0 = \int d^4x \overline{\psi}(x)\Big[\gamma_\mu D_\mu + M_{\mathrm{R}}\Big]\psi(x), \qquad \text{with} \qquad M_{\mathrm{R}} = Z_{\mathrm{M}}(g_0^2, a\mu)M \tag{5.12}$$

To understand how the choice of a twisted Wilson term influences the Ward identities of the theory we rewrite some of them in the physical basis. To deduce them it is enough to start from the Ward identities in the twisted basis, where using a mass independent renormalization scheme, one can make a standard analysis to construct the lattice fields that are multiplicatively renormalizable and respect, up to cutoff

effects, the chiral multiplet structure. The final step is then to rotate all the quark fields back into the physical basis.

Renormalized vector and axial currents can be taken to be

$$(\mathcal{V}_{\rm R})^a_\mu = Z_A\,\mathcal{V}^a_\mu \qquad (\mathcal{A}_{\rm R})^a_\mu = Z_V\,\mathcal{A}^a_\mu \qquad a = 1,2\,, \tag{5.13}$$

$$(\mathcal{V}_{\rm R})^3_\mu = Z_V\,\mathcal{V}^3_\mu \qquad (\mathcal{A}_{\rm R})^3_\mu = Z_A\,\mathcal{A}^3_\mu, \tag{5.14}$$

where the local currents in the physical basis are defined in eqs. (2.12,2.13) and the finite renormalization constants, Z_V and Z_A, are those for the local vector and axial currents of standard Wilson fermions, respectively. Notice the switch between Z_V and Z_A for the currents with flavour $a = 1, 2$, due to the presence of the factor $\gamma_5\tau_3$ in front of the Wilson term in eq. (5.4).

The expressions for the renormalized densities are

$$\mathcal{P}^a_{\rm R} = Z_P\,\mathcal{P}^a \qquad \mathcal{P}^3_{\rm R} = Z_{S^0}\Big[\mathcal{P}^3 + \frac{i\rho_P(aM)}{a^3}\Big], \tag{5.15}$$

$$\mathcal{S}^0_{\rm R} = Z_P\Big[\mathcal{S}^0 + \frac{M\rho_{S^0}(aM)}{a^2}\Big] \tag{5.16}$$

where $\rho_P(aM)$ is a polynomial in aM, while $\rho_{S^0}(aM)$ is a polynomial with even powers of aM. The reason for this is because $\widetilde{\mathcal{R}}^{1,2}_5$ is a symmetry of the lattice action (5.11). Formula (5.16) is rather interesting because it shows that the chiral order parameter is only affected by an M/a^2 power divergence, analogously to what happens with Ginsparg-Wilson fermions.

The non-singlet Ward identities (2.20), once the local operators are properly renormalized, are valid at fixed lattice spacing up to cutoff effects

$$\partial^*_\mu\langle(\mathcal{V}_{\rm R})^a_\mu(x)\mathcal{O}_{\rm R}(y)\rangle = 0 \tag{5.17}$$

$$\partial^*_\mu\langle(\mathcal{A}_{\rm R})^a_\mu(x)\mathcal{O}_{\rm R}(y)\rangle = 2M_{\rm R}\langle\mathcal{P}^a_{\rm R}(x)\mathcal{O}_{\rm R}(y)\rangle \tag{5.18}$$

with $\mathcal{O}$ being a generic multilocal operator and $x \neq y$.

5.2 Automatic O(a) improvement

In this section we are going to prove again automatic O(a) improvement in the physical basis in infinite volume.

The target continuum theory for the fermion fields will be now

$$S_0 = \int d^4x\overline{\psi}(x)\Big[\gamma_\mu D_\mu + M_{\rm R}\Big]\psi(x), \tag{5.19}$$

The Symanzik effective action in eq. (4.3) now has correction terms given by

$$S_1 = \int d^4y \mathcal{L}_1(y) \qquad \mathcal{L}_1(y) = \sum_i c_i \mathcal{O}_i(y), \tag{5.20}$$

with operators of the form

$$\mathcal{O}_0 = i\Lambda^2 \overline{\psi}\gamma_5\tau^3\psi, \qquad \mathcal{O}_1 = i\overline{\psi}\gamma_5\tau^3\sigma_{\mu\nu}F_{\mu\nu}\psi, \qquad \mathcal{O}_5 = iM^2\overline{\psi}\gamma_5\tau^3\psi. \tag{5.21}$$

where Λ is an energy scale of the order of the QCD scale $\Lambda_{\rm QCD}$. The operator $\mathcal{O}_1$ is the usual clover term in the physical basis, where the Wilson term is chirally rotated. The operator $\mathcal{O}_0$ parametrizes the unavoidable mass independent O(a) uncertainties in the critical mass.

We can now repeat the same steps followed in sect. 4. We consider a general multiplicatively renormalizable multilocal field that in the effective theory is represented by the effective field

$$\Phi_{\rm eff} = \Phi_0 + a\Phi_1 + \dots \tag{5.22}$$

A lattice correlation function of the field Φ to order a is given by

$$\langle\Phi\rangle = \langle\Phi_0\rangle_0 - a\int d^4y \langle\Phi_0\mathcal{L}_1(y)\rangle_0 + a\langle\Phi_1\rangle_0 + \dots \tag{5.23}$$

where the expectation values on the r.h.s are to be taken in the continuum theory with action S_0. The key point is that the continuum action (5.19) is symmetric under isovector flavour transformations. In particular the discrete flavour rotations

$$\mathcal{F}^{1,2}\colon \begin{cases} \psi(x_0,\mathbf{x}) \to i\tau^{1,2}\psi(x_0,\mathbf{x}) \\ \overline{\psi}(x_0,\mathbf{x}) \to -i\overline{\psi}(x_0,\mathbf{x})\tau^{1,2} \end{cases} \tag{5.24}$$

are symmetries of the continuum action. On the contrary all the operators in eq. (5.21), of the Symanzik expansion of the lattice action, are odd under the the discrete flavour symmetry (5.24). If the field Φ is a lattice representation of the flavour even field Φ_0 then the second term in the r.h.s. of eq. (5.23) vanishes. To show that also the Φ_1 term vanishes we have to show that an operator of one dimension higher than the original one but the same lattice symmetries has opposite discrete flavour number. This goes exactly in the same way as in the twisted basis (see sect. 4). The gauge action is invariant under the symmetry [11]

$$\widetilde{\mathcal{D}} = \mathcal{D} \times [M \to -M] \tag{5.25}$$

where

$$\mathcal{D}\colon \begin{cases} U(x;\mu) \to U^\dagger(-x - a\hat{\mu};\mu), \\ \chi(x) \to \mathrm{e}^{3i\pi/2}\chi(-x) \\ \overline{\chi}(x) \to \overline{\chi}(-x)\mathrm{e}^{3i\pi/2}, \end{cases} \tag{5.26}$$

while in the fermion action the terms that break flavour symmetry $\mathcal{F}^{1,2}$ symmetry are odd. But in particular the lattice action is invariant under $\mathcal{F}^{1,2} \times \widetilde{\mathcal{D}}$. So the operators in Φ_1 will necessarily have opposite flavour number to Φ_0. Given the fact that the continuum action is flavour symmetric also Φ_1 vanishes. Possible contact terms coming from the second term amount to a redefinition of Φ_1 as we have discussed in sec. 4 and so do not harm the proof.

The same proof can be repeated using the parity symmetry $\mathcal{P}$ defined in eq. (2.34) instead of using the discrete flavour symmetry $\mathcal{F}^{1,2}$.

6 O(a^2) cutoff effects

In this section I will be mainly concerned with the O(a^2) cutoff effects of the Wtm formulation and in particular on the cutoff effects induced by the breaking of flavour and parity symmetry. Some of these require a formal description of the quantum mechanical representation for a lattice correlator computed with the Wtm action. The first part of this section will be devoted to a brief introduction of the basic Hamiltonian formalism, while the second part will be concentrated on the typical consequences of these breaking effects on physical observables. A third part will deal with a possible strategy in order to attenuate these O(a^2) effects.

6.1 Hamiltonian formalism

We assume we are in a finite volume L, which is large enough to consider hadronic states as point-like. This is likely to be the situation for the actual lattice simulations with 2fm $\lesssim L \lesssim$ 4fm. The relation among euclidean correlation function, hadron masses and matrix elements is given in the Hamiltonian formalism by the transfer matrix of the lattice theory. We have shown in sect. 2 that for Wtm the transfer matrix exists and it is positive definite. As a consequence of physical positivity a lattice correlation function admits a quantum mechanical representation in term of states belonging to the Hilbert space of the theory. This complete set of states can be chosen to be the eigenstates $|n, q\rangle$ of the Hamiltonian $\mathbb{H}$

$$\mathbb{H}|n,q\rangle = E_n^{(q)}|n,q\rangle \ , \qquad \mathbb{1} = \sum_{n,q} |n,q\rangle\langle n,q| \tag{6.1}$$

where q indicates a set of the quantum numbers corresponding to the symmetries of the lattice action and n the energy level given a certain quantum number. We choose here the following normalization

$$\langle n',q'|n,q\rangle = 2E_n^{(q)}\delta_{n',n}\delta_{q',q} \tag{6.2}$$

The set of quantum numbers that it is possible to use to classify the states for Wtm are $q \equiv \{j, P_F^1, C, Q_3, \mathbf{p}\}$ corresponding to the symmetries of Wtm: charge conjugation $\mathcal{C}$, parity combined with flavour exchange $\mathcal{P}_F^1$, charge associated to the residual $U_{\rm V}(1)_3$ flavour symmetry Q_3, the representation of the $H(3)$ group of spatial discrete rotations j and the spatial momentum $\mathbf{p}$ [15] .

In the case of plain Wilson fermions (eq. 2.28 with $\mu_{\rm q} = 0$) we could replace $\mathcal{P}_F^1$ and Q_3 with standard parity and isospin symmetry $\mathcal{P}$, I and I_3. For Wtm the set of quantum numbers q is smaller than in the continuum. This means that certain states that

[15] $\mathcal{P}_F^2$ is not used because it is not independent from $\mathcal{P}_F^1$ and Q_3.

in the continuum have different quantum numbers, cannot be disentangled anymore with Wtm. A typical example is the neutral pion where we have $q_{\pi^0} = \{j, +, +, 0, \mathbf{0}\}$ that is certainly not distinguishable from the vacuum. More generally in the quantum mechanical representation of the correlation functions computed with Wtm, there will be parity violating matrix elements which vanish only in the continuum limit. Even if technically this is slightly more complicated that analyzing correlators in the plain Wilson case, the state of art for the analysis of correlation functions requires a multi-state fit, which is what we need to extract the masses and matrix elements we are interested in. Moreover given the fact that these matrix elements vanish in the continuum limit, it could be that numerically these contributions are very small at sufficiently fine lattices. To be specific I will concentrate here on 2 examples in order to show how to proceed.

6.2 Pion channel correlator

We take here a finite 4–d lattice with spacing a. We want to write the quantum mechanical decomposition of the following correlator

$$C^{11}_{\rm PP}(x_0) = -a^3 \sum_{\mathbf{x}} \langle P^1(x_0, \mathbf{x}) P^1(0) \rangle \ . \tag{6.3}$$

Since we sum over $\mathbf{x}$, only states with vanishing spatial momentum contribute. Moreover we concentrate on the trivial representation of H(3) and since we neglect electromagnetic interactions it is more convenient to study eigenstates of charge conjugation $\mathcal{C}$. The relevant quantum numbers are the quantum numbers of the charged and neutral pion

$$q_{\pi^1} = \{0, -, +, 1, \mathbf{0}\} \ , \qquad q_{\pi^0} = \{0, +, +, 0, \mathbf{0}\} \ . \tag{6.4}$$

The eigenstates of charge conjugation are

$$|0, \pi^1(\mathbf{p})\rangle = \frac{1}{\sqrt{2}}(|0, \pi^+(\mathbf{p})\rangle + |0, \pi^-(\mathbf{p})\rangle) \qquad |0, \pi^2(\mathbf{p})\rangle = \frac{-i}{\sqrt{2}}(|0, \pi^+(\mathbf{p})\rangle - |0, \pi^-(\mathbf{p})\rangle) \ . \tag{6.5}$$

These two states have the same mass because of the residual $U_{\rm V}(1)_3$ isospin symmetry. Using the standard representation of a correlation function in terms of the local operators $\hat{P}^1$, and inserting a complete set of states, we obtain (for simplicity we consider the lattice time extent $T \to \infty$)

$$C^{11}_{\rm PP}(x_0) = \frac{1}{\mathcal{Z}} \sum_{n,q} \langle 0, \Omega | \hat{P}^1 | n, q \rangle \frac{e^{-E^{(q)}_n x_0}}{2E^{(q)}_n} \langle n, q | \hat{P}^1 | 0, \Omega \rangle \ . \tag{6.6}$$

A detailed analysis of the excited states can become rather involved. Here we concentrate on the fundamental and the first excited state which is a specific contribution

of Wtm

$$n = 0 \Rightarrow |0, \pi^1(\mathbf{0})\rangle \tag{6.7}$$

$$n = 1 \Rightarrow |1, \pi^1(\mathbf{0})\pi^0(\mathbf{0})\rangle. \tag{6.8}$$

We are here implicitly assuming that in the chosen volume L the energy level of the two pion state with zero relative momentum is well separated from the energy levels of the excited two pion state. From fig. 1 of ref. [92] this seems to be certainly the case for the volumes which are currently simulated.

Contrary to what happens with standard Wilson fermions, the first excited state is given by a two pion contribution. The parity symmetry of the the continuum QCD action implies that the matrix element $|\langle 0, \Omega|\hat{P}^1|1, \pi^1\pi^0\rangle|$ must vanish in the continuum limit. This means it is at most an $\mathrm{O}(a)$ term. This implies that the amplitude $|\langle 0, \Omega|\hat{P}^1|1, \pi^1\pi^0\rangle|^2$ is an $\mathrm{O}(a^2)$ effect independently of whether we set the untwisted quark mass to zero or not [16]. The first two terms of eq. (6.6) read

$$\begin{aligned} &|\langle 0, \Omega|\hat{P}^1|1, \pi^1(\mathbf{0})\rangle|^2 \frac{e^{-M_{\pi^1} x_0}}{2M_{\pi^1}} \times \\ &\times \left\{ 1 + \frac{|\langle 0, \Omega|\hat{P}^1|1, \pi^1(\mathbf{0})\pi^0(\mathbf{0})\rangle|^2}{\langle 0, \Omega|\hat{P}^1|1, \pi^1(\mathbf{0})\rangle|^2} e^{-\left(E_{2\pi}(L) - M_{\pi^1}\right)x_0} \frac{M_{\pi^1}}{E_{2\pi}(L)} + \ldots \right\}, \end{aligned} \tag{6.9}$$

where $E_{2\pi}(L)$ represents the lowest energy level for the two pion state. At finite lattice spacing a the excited state correction increases when the quark mass goes to zero. In fact, up to finite size corrections, the gap is proportional to the neutral pion mass which, as we will see in sects. 6.4.1 and 6.5.1, vanishes at very small values of the twisted mass. This could be in principle a problem for a reliable extraction of the charged pion mass. Practically the problem is absent because $|\langle 0, \Omega|\hat{P}^1|1, \pi^1\pi^0\rangle|^2$ is of $\mathrm{O}(a^2)$ and, like all the other parity violating contributions to the correlator, it is highly suppressed at sufficiently small lattice spacing. An additional suppression factor is given by $\frac{M_{\pi^1}}{E_{2\pi}(L)}$. We remark that, independently on the lattice QCD formulation used, the gap between the fundamental and the first excited state in the pion channel will always go to zero in large volumes, because the first excited state will be at most a 3 pions state with vanishing momentum.

Since Wtm does not preserve parity at finite lattice spacing, it would be possible in principle to have as excited state a charged scalar. But the scalar that can be created must have opposite isospin component because parity "times" isospin in direction 1 and 2 ($\mathcal{P}_F^{1,2}$, defined in eq. 2.38) is a symmetry of the lattice action. This isospin component of the scalar current has opposite charge conjugation. The residual $U_{\mathrm{V}}(1)_3$ symmetry (2.40) excludes mixing with the remaining isospin components of the scalar particle.

[16] I acknowledge very useful discussions with G. Herdoiza and R. Frezzotti on this point.

The conclusion of this discussion is that the first excited state contributions typical of Wtm are either absent, like the charged scalar, or highly suppressed like the two pion state. This is nicely confirmed by the recent unquenched simulations performed by the ETM Collaboration [93]. In fig. 9, I show a typical effective mass for $N_f = 2$ dynamical quarks. A long plateau in euclidean time is observed that allows a very precise determination of the pseudoscalar mass. We conclude that Wtm does not seem to make more difficult extracting the pseudoscalar mass, compared with other lattice actions which preserve parity symmetry.

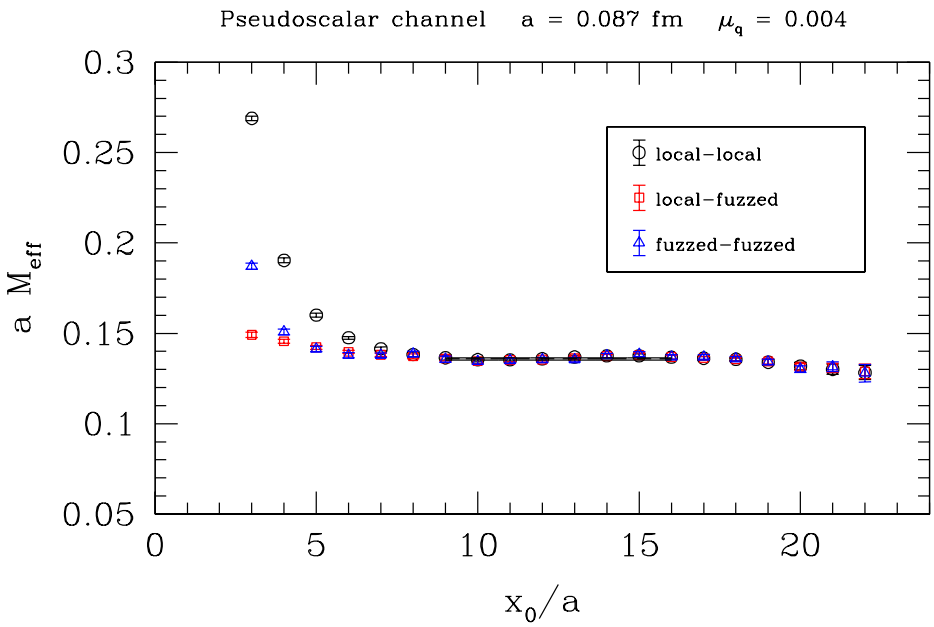


Fig. 9. Effective mass for the pseudoscalar channel for a lattice spacing of $a = 0.087$ fm and a corresponding mass of 292 MeV. The masses using 3 different interpolating operators are shown.

6.3 Charged scalar channel correlator

The same analysis can be repeated for the charged scalar correlator. In particular we want to study the correlator for the charged a_0 scalar meson. The relevant quantum numbers are

$$q_{a_0^1} = \{0, +, +, 1, \mathbf{0}\} \ , \qquad q_\eta = \{0, -, +, 0, \mathbf{0}\} \ . \tag{6.10}$$

The η we consider here is the pseudoscalar isosinglet in the $SU(2)$ framework, sometimes labelled as η_2. The leading contributions of the charged scalar correlator

$$C^{11}_{\rm SS}(x_0) = \frac{1}{\mathcal{Z}} \sum_{n,q} \langle 0, \Omega | \hat{S}^1 | n, q \rangle \frac{e^{-E_n^{(q)} x_0}}{2E_n^{(q)}} \langle n, q | \hat{S}^1 | 0, \Omega \rangle \ , \tag{6.11}$$

are

$$n = 0 \Rightarrow |0, a_0^1(\mathbf{0})\rangle \tag{6.12}$$

$$n = 1 \Rightarrow |1, a_0^1(\mathbf{0})\pi^0(\mathbf{0})\rangle, \qquad |1, \eta(\mathbf{0})\pi^1(\mathbf{0})\rangle. \tag{6.13}$$

The $|1, \eta\pi^1\rangle$ state is the natural decay channel for the charged scalar particle. If the values of the quark masses in the simulations are such that the decay threshold is not open, this term contributes as an excited state with a gap from the fundamental state which could be very small.

The parity violating term in the spectral decomposition is, analogously to the pseudoscalar channel, proportional to

$$\frac{|\langle 0, \Omega|\hat{S}^1|1, a_0^1(\mathbf{0})\pi^0(\mathbf{0})\rangle|^2}{|\langle 0, \Omega|\hat{S}^1|0, a_0^1(\mathbf{0})\rangle|^2} \mathrm{e}^{-\left(E_{a_0\pi}(L) - M_{a_0}\right)x_0}, \tag{6.14}$$

with an amplitude squared of $\mathrm{O}(a^2)$.

In fig. 10 we see an example of a charged scalar correlator, from a recent analysis of $N_f = 2$ dynamical configurations [93].

Using the same argument we have use in the previous section to exclude a charged scalar as a possible excited state of the charged pseudoscalar, we can exclude the presence of a single pion intermediate state. As a confirmation of this fact there is no sign in fig. 10 that the correlator dips down to the value of the pseudoscalar mass.

6.4 Isospin violation

The fact that Wtm at finite lattice spacing breaks isospin symmetry, while retaining the isovector subgroup $U_{\mathrm{V}}(1)_3$, allows a splitting between neutral and charged pions. This is not a physical splitting and in the continuum limit of a $N_{\mathrm{f}} = 2$ theory with degenerate quarks we will obtain again a degenerate triplet of pions (if we neglect, as we do here, the electromagnetic interactions). But at finite lattice spacing the masses of the charged and neutral pion are not the same. This is a very important issue to understand and rather surprisingly only recently numerical simulations started to investigate this issue [71,94,95]. Other examples of isospin violating cutoff effects are the splitting in the kaon sector or in the Δ-baryon multiplet investigated numerically in [68]. In general the isospin splitting is an $\mathrm{O}(a^2)$ effect independently of the value of the twist angle. This can be shown using the symmetry $\mathcal{P}_F^{1,2}$ (2.38) which is the product of parity and flavour exchange. This is a symmetry of Wtm (2.28) independently on the value of the twist angle. This symmetry of the lattice action implies that all the dimension 5 counterterms of the Symanzik effective action will have to be even under $\mathcal{P}_F^{1,2}$. For parity conserving correlation functions this automatically

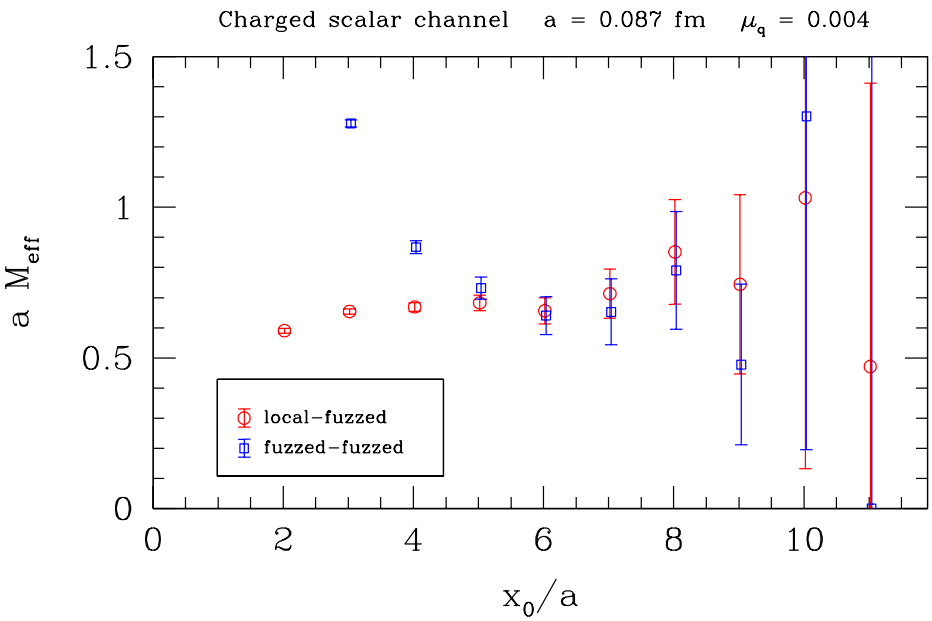


Fig. 10. The same as fig. 9 but for the charged scalar channel and with the two best correlators.

implies that their $O(a)$ insertion will contribute in the same way to the correlation functions independently on their flavour structure. Thus the isospin splitting has to be at least of $O(a^2)$ independently on the value of the twist angle. In other words the $O(a)$ affecting the neutral and charged pion correlation functions out of full twist are the same. This is confirmed by the results obtained in WχPT [83,96] and discussed in the following section.

6.4.1 Pion splitting

To fix the notation we recall some basic definitions. The charged pseudoscalar densities are given by

$$P^{\pm}(x) = \overline{\chi}(x)\gamma_5\tau^{\pm}\chi(x) \qquad \tau^{\pm} = \frac{\tau^1 \pm \mathrm{i}\tau^2}{2} \tag{6.15}$$

and a possible interpolating field for the neutral pion, with $\omega = \pi/2$, is the scalar current

$$\frac{1}{\sqrt{2}}S^0(x) = \frac{1}{\sqrt{2}}\overline{\chi}(x)\chi(x). \tag{6.16}$$

The charged and neutral pseudoscalar masses can be extracted by the following correlators

$$C_{\pi^+}(x_0) = -a^3 \sum_{\mathbf{x}} \langle P^+(x) P^-(0) \rangle \qquad C_{\pi^0}(x_0) = \frac{a^3}{2} \sum_{\mathbf{x}} \langle S^0(x) S^0(0) \rangle. \tag{6.17}$$

If we separate the flavour components and we perform the fermionic contractions we obtain

$$\begin{aligned} C_{\pi^0}(x_0) = \frac{a^3}{2} \sum_{\mathbf{x}} \Big\{ \Big\langle & -\mathrm{tr}\Big[G_u(0,x) G_u(x,0)\Big] - \mathrm{tr}\Big[G_d(0,x) G_d(x,0)\Big] \\ & + \mathrm{tr}\Big[G_u(x,x)\Big] \mathrm{tr}\Big[G_u(0,0)\Big] + \mathrm{tr}\Big[G_u(x,x)\Big] \mathrm{tr}\Big[G_d(0,0)\Big] \\ & + \mathrm{tr}\Big[G_d(x,x)\Big] \mathrm{tr}\Big[G_u(0,0)\Big] + \mathrm{tr}\Big[G_d(x,x)\Big] \mathrm{tr}\Big[G_d(0,0)\Big] \Big\rangle \Big\} \end{aligned} \tag{6.18}$$

where $G_{u,d}(x,y)$ are the fermionic propagators for the the *up* and *down* quarks.

The neutral pion correlator (6.18) contains fermionic disconnected diagrams (the last four terms in eq. 6.18), which are notoriously more difficult to compute on the lattice. One way to circumvent this problem is to consider only the fermionic connected part (the first two terms of eq. 6.18). The question would be now if it is still possible to interpret the fermionic connected piece as coming from a correlation function between local operators which represent a pion field. The answer is positive if we consider the valence quarks of the theory discretized with the so called Osterwalder-Seiler (OS) action [97, 98]. To be specific we consider now the following model: the sea quarks are described by the standard $N_f = 2$ degenerate Wtm action (2.28) while the valence quarks, that we call u and d' have the following actions

$$S_{\mathrm{OS}}^{(u)} = a^4 \sum_x \Big\{ \bar{u}(x) \left[D_{\mathrm{W}} + m_{\mathrm{cr}} + i\mu_u^v \gamma_5 \right] u(x) \Big\}. \tag{6.19}$$

$$S_{\mathrm{OS}}^{(d')} = a^4 \sum_x \Big\{ \bar{d}'(x) \left[D_{\mathrm{W}} + m_{\mathrm{cr}} + i\mu_{d'}^v \gamma_5 \right] d'(x) \Big\}. \tag{6.20}$$

These two quarks have the same mass $\mu_u^v = \mu_{d'}^v$, thus they have identical actions, differing only because they have different flavours. We can then define as interpolating field for the neutral pion

$$(\pi^0)'(x) = \frac{1}{\sqrt{2}} \Big[\bar{u}(x) u(x) - \bar{d}'(x) d'(x) \Big]. \tag{6.21}$$

It is easy to see that, performing the axial rotations (2.6) corresponding to the actions (6.19,6.20)

$$\begin{cases} u(x) \longrightarrow \exp(-i\frac{\omega}{2}\gamma_5) u(x) \\ \bar{u}(x) \longrightarrow \bar{u}(x) \exp(-i\frac{\omega}{2}\gamma_5), \end{cases} \qquad \begin{cases} d'(x) \longrightarrow \exp(-i\frac{\omega}{2}\gamma_5) d'(x) \\ \bar{d}'(x) \longrightarrow \bar{d}'(x) \exp(-i\frac{\omega}{2}\gamma_5), \end{cases} \tag{6.22}$$

with $\omega = \pi/2$, this is a valid interpolating field for the neutral pion. Performing standard Wick contractions we obtain

$$C_{(\pi^0)'}(x_0) = a^3 \sum_{\mathbf{x}} \Big\{ \Big\langle -\mathrm{tr}\Big[G_u(0,x)G_u(x,0)\Big] - \mathrm{tr}\Big[G_{d'}(0,x)G_{d'}(x,0)\Big]\Big\rangle \Big\}, \qquad (6.23)$$

where the disconnected terms cancel because the u and d' quarks have identical propagators. Since parity "times" flavour exchange is a symmetry of the lattice action we have

$$\gamma_0 G_d(0,x_{\mathrm{P}})\gamma_0 = G_u(0,x) = G_{d'}(0,x), \qquad \text{with} \quad x_{\mathrm{P}} = (x_0, -\mathbf{x}). \qquad (6.24)$$

The connected part of the neutral pion correlator with Wtm (6.18) is equal to the correlation function (6.23) for a model with OS valence quarks. This argument tells us that the connected part of eq. (6.18) is not the π^0 propagator with Wtm, but it is still a π^0 propagator with valence quarks having the same OS actions (6.19,6.21). In the continuum limit the two neutral pion correlators will coincide.

The OS action can be used only as a discretization for valence quarks because a parity violating and isospin singlet counterterm like $F\tilde{F}$ could be otherwise generated in the process of renormalizing the theory (see sect. 2). This freedom of choosing a different lattice action between valence and sea quarks will be further used to ease the renormalization of local operator (see sect. 7). Here we just use this freedom as a tool to interpret the fermionic connected part as a theoretically valid expression of a correlation function between local operators. We remark that the fermionic connected part is *not* the neutral pseudoscalar meson of Wtm, but it is an interesting quantity to study with precise data on its own, in view of a possible use of mixed actions (the OS action for the valence quarks and Wtm for the sea quarks). Moreover in the quenched model the fermionic determinant is neglected anyhow, and this puts the two models (quenched OS and quenched Wtm) on the same footing.

We also note that in the same model we could define a charged pion made up of a u and d' quark. In this case the correct interpolating field would be $\bar{u}d'$ that has identical correlation function with the neutral pion field $(\pi^0)'$. This leads to a model with NO isospin splitting among the pions. The drawback of this choice would be, apart from $\mathrm{O}(a^2)$ unitarity violations, that this charged pion field is not the field that is protected by the exact lattice Ward identity (7.2).

The choice of valence actions different from the sea action allows freedom to solve some problems which appear in the unitary formulation. We will see in sect. 7 how this freedom can simplify the renormalization of local operators. It remains to be seen how the $\mathrm{O}(a^2)$ unitarity violations affect the theory and the approach to the continuum limit. This is an open question which could be answered only performing detailed scaling tests.

In [94], to which I refer for all the technical details, a pilot quenched study has been performed to study flavour breaking effects with Wtm. In this paper the scaling behaviour is studied in the quenched model of the pion splitting using either only the connected correlator $((M^0_{\rm PS})^2_{\rm OS} - (M^+_{\rm PS})^2)$, or including also the disconnected terms $((M^0_{\rm PS})^2 - (M^+_{\rm PS})^2)$ [17] . The results show $O(a^2)$ scaling violations for both the pion splittings with indications that the neutral pseudoscalar meson for Wtm (with the inclusion of the disconnected correlator) has reduced splitting with the charged meson, within the rather large statistical errors. It is possible to give a very rough estimate of the pion splitting $r_0^2((M^0_{\rm PS})^2 - (M^+_{\rm PS})^2) \simeq c(a/r_0)^2$ with $c \simeq 10$ (with large errors). Comparing to a quenched simulation for naïve staggered fermions with Wilson gauge action [99], one finds a similar size of the flavour splitting encountered for the pion mass at a similar lattice spacing with a value $c \simeq 40$. For dynamical improved staggered fermions a value of $c \simeq 10$ has been found [100].

The pion splitting has been investigated in the quenched model in [71], where a comparison between the impact on the methods used to determine the critical mass has been made. The outcome of this study is that if one considers only the fermionic connected diagrams (OS neutral pion) the inclusion of the clover term into the Wtm lattice action (4.18) reduces the pion splitting in comparison with the Wtm action without clover term. This result is rather interesting but not conclusive, in fact the addition of the disconnected terms can have a tremendous impact as we have just seen in the quenched model. Moreover recent dynamical simulations [69] indicate that the inclusion of the disconnected terms changes the sign of the pion-splitting. To be precise the outcome is that a first analysis at a value the pseudoscalar mass $M_{\rm PS} \simeq 300$ MeV, taking the disconnected contribution in the neutral channel fully into account, shows that the neutral pseudoscalar meson is about 20% lighter than the charged one. Expressed differently one obtains $r_0^2((M^0_{\rm PS})^2 - (M^+_{\rm PS})^2) = c(a/r_0)^2$ with $c = -4.5(1.8)$. This coefficient is, in absolute value, a factor of 2 smaller than the value found in quenched investigations [101]. If one considers only the connected term, i.e. considering OS valence quarks, the charged pion is lighter or in other words the sign of c is positive.

From the theoretical side a tool to address and understand this problem is again WχPT. Adopting the same power counting scheme used in sect. 4 given in eq. (4.67) the result [83, 96] at NLO order is

$$M^2_{\pi^0} - M^2_{\pi^\pm} = -2a^2 w' \frac{\mu_{\rm R}^2}{m'^2 + \mu_{\rm R}^2} \,. \tag{6.25}$$

The splitting is as expected an $O(a^2)$ effect and vanishes on the Wilson axis ($\mu_{\rm R} = 0$) as it should. It is moreover necessarily even in $\mu_{\rm q}$, from the combined violation of

[17] In both computations the "PCAC method" is used for the determination of the critical mass.

parity and isospin argument given in sect. 6.4. The splitting is maximized when $m' = 0$ as it should be since this is the condition that minimizes the parity violation. The sign of the LEC w' tells us which pion is heavier. We will see in sect. 6.5 that w' also determines the nature of the vacuum structure of the theory around the chiral point.

Given the non-degeneracy among the pion multiplet, several issues would have to be investigated in the future. The usage of a mixed action approach with OS valence quarks (or another isospin conserving action like the overlap discretization) eliminates the problem of isospin splitting at the valence level. Of course the isospin breaking cutoff effects of the sea Wtm action will still generate a splitting, but only among the virtual pions. One possible consequence of this phenomenon is the change of the finite size effects in a physical quantity induced by the pion cloud: the dominant contribution comes from the lightest pion of the theory at finite lattice spacing, that, as we have seen, is not necessarily the charged one [18] .

6.4.2 Kaon splitting

With an interest in the phenomenology of hadrons built of u, d and s quarks, it is useful to explore Wtm including heavier quarks. We have already seen in sect. 2 that there is no unique way to introduce the s quark into the calculation. The method investigated in ref. [95] considers a pair of quark doublets (u, d) and $(\text{“}c\text{”}, s)$, following the proposal of ref. [39] discussed in sect. 3.2. In particular the partner of the s quark does not play an active role and should not be thought of as the physical charm quark; moreover with this method no mass splitting is introduced within either doublet.

To be specific one introduces Wtm with two degenerate quark doublets,

$$\chi_l = \begin{pmatrix} u \\ d \end{pmatrix} , \qquad \chi_h = \begin{pmatrix} c \\ s \end{pmatrix} , \tag{6.26}$$

referred to as the light and heavy doublets respectively.

As we have seen in sect. 2 this construction can be extended to include non-degenerate quarks in a single doublet [39]. Even if with this approach the fermion determinant is not real, and so it would not be practical to perform dynamical simulations, this action could still be useful in the spirit of using different lattice actions for the valence and the sea quarks.

The two-doublet lattice action is simply a block-diagonal version of two copies of

[18] I thank C. Michael for bringing also my attention to this issue.

the one-doublet theory (2.28).

$$S_F^L = a^4 \sum_x \overline{\chi}(x) \Big[\frac{1}{2} \sum_\mu \gamma_\mu (\nabla_\mu^\star + \nabla_\mu) - \frac{a}{2} \sum_\mu \nabla_\mu^\star \nabla_\mu + \boldsymbol{m} + i\gamma_5 \boldsymbol{\mu} \Big] \chi(x) \,, \qquad (6.27)$$

where ∇_μ and $\nabla_\mu^\star$ are the usual covariant forward and backward lattice derivatives respectively, and

$$\chi = \begin{pmatrix} \chi_l \\ \chi_h \end{pmatrix} \,, \qquad \boldsymbol{m} = \begin{pmatrix} m_{l,\,0}\, \mathbb{1}_2 & 0 \\ 0 & m_{h,\,0} \mathbb{1}_2 \end{pmatrix} \,, \qquad \boldsymbol{\mu} = \begin{pmatrix} \mu_{l,\,\mathrm{q}} \tau_3 & 0 \\ 0 & \mu_{h,\,\mathrm{q}} \tau_3 \end{pmatrix} \,. \qquad (6.28)$$

The method used in [95] to fix the critical mass is the "ω_A method", with the untwisted bare quark mass tuned so as to achieve full twist at each particular twisted mass value.

NLO WχPT [95] predicts a formula for $M^2_{\mathrm{K}^0} - M^2_{\mathrm{K}^\pm}$ very similar to the formula for the pion splitting (6.25). In particular this formula, analogously to the pion case, predicts for the kaon splitting at NLO no dependence on the twisted quark mass if the twist angles for the light and the heavy sector are $\omega = \pi/2$ for all the values of the twisted mass ("ω_{A} method"). The same formula, again analogously to the pion case, predicts that the kaon splitting should depend linearly in a^2 and it should vanish in the continuum limit. Modulo the unknown higher order effects, figs. 11 and 12 are in reasonable agreement with these expectations. In fig. 11 are plotted the masses squared of the charged and neutral kaons, *i.e.* the ground state pseudoscalar mesons containing one s quark from the heavy doublet and one u or d quark from the light doublet, as a function of the sum of the valence twisted quark masses. Fig. 12 shows the lattice spacing dependence of the squared mass differences for four mass values. To summarize: the approximate mass independence of the kaon splitting is evident from fig. 11, and the dependence on a^2 in fig. 12 is approximately linear, though a linear fit misses the massless prediction at $a = 0$ by a few (statistical) standard deviations.

It should be noted from fig. 12 that even at the smallest lattice spacing, the mass splitting of $m_{K^0} - m_{K^\pm} \sim 50$ MeV is significant relative to the kaon mass itself. However, in terms of the difference of mass squared, these results are consistent with the pseudoscalar meson mass splittings discussed in ref. [94].

The splitting in the Kaon system that we have just discussed involves only twisted quarks. Different $\mathrm{O}(a^2)$ cutoff effects appear if one studies the splitting between pseudoscalar correlators computed with twisted and untwisted quarks. One can consider a twisted (u, d) doublet, and flavour-singlet Wilson strange (and charm) quarks. This approach could be a viable one for doing full dynamical simulations. On the other side automatic $\mathrm{O}(a)$ improvement would be lost and there would be the need

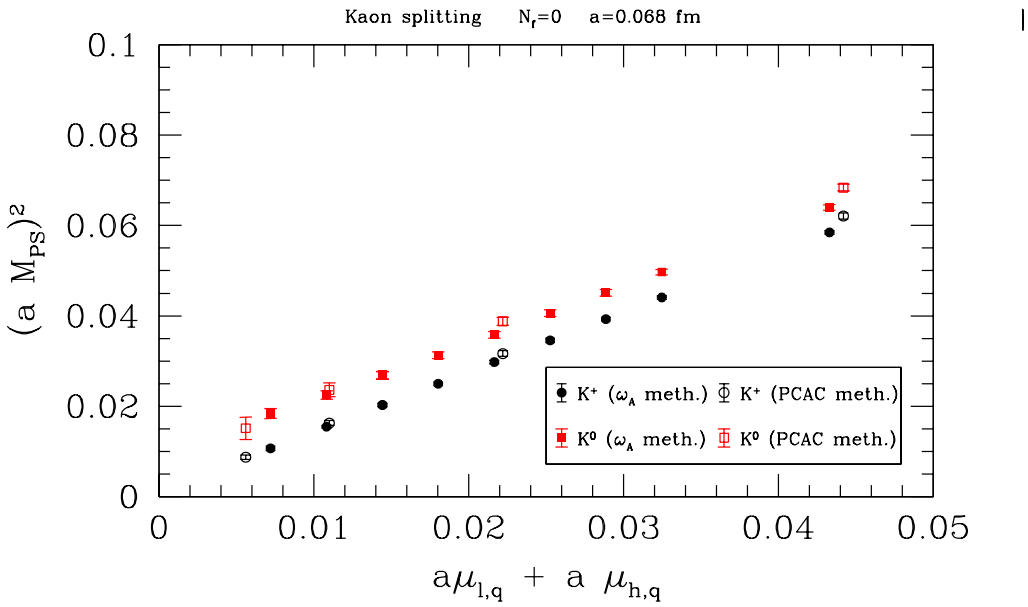


Fig. 11. Pseudoscalar meson mass squared as a function of the sum of quark and antiquark twisted mass parameters. Subscripts l and h indicate the light and heavy doublets. Results are taken from ref. [95] which uses the ω_A method and and from ref. [94] which uses the PCAC method. The results from [94] have equal masses for the quark and anti-quark.

to introduce suitable improvement coefficients. In ref. [72] a precise investigation has been performed, in the quenched model, of this particular splitting between pseudoscalar correlators induced by the fact that twisted and untwisted actions have been used for the quarks. The twisted and untwisted actions of [72] are both clover improved, and all the relevant improvement coefficients have been used to improve the correlators. The twisted and untwisted quark masses are always matched in order to have the same continuum QCD theory with meson masses around the Kaon mass. The critical mass $m_{\rm cr}$ used in [72] has been taken from refs. [43,73,74] and it has been recomputed at one lattice spacing. The quantities studied in this paper are the pseudoscalar masses $M_{\rm tt}$, $M_{\rm tW}$, $M_{\rm WW}$ and decay constants $F_{\rm tt}$, $F_{\rm tW}$, $F_{\rm WW}$ for mesons which are respectively made of a doublet of twisted quarks tt, a twisted and untwisted quark tW and two untwisted quarks WW. The meson made of twisted quarks is the charged pseudoscalar correlator of eq. (6.17). The outcome of this precise quenched study is that the splitting between pseudoscalar meson masses and decay constants ranges, at the coarsest lattice spacing $a = 0.093$ fm, between 5-13% and it goes to zero in the continuum limit. The splitting seems to depend also on the value of the improvement coefficient $c_{\rm A}$ which is needed to improve the axial current with Wilson fermions. In this paper the issue of the pseudoscalar splitting induced by the twisted mass term is not addressed.

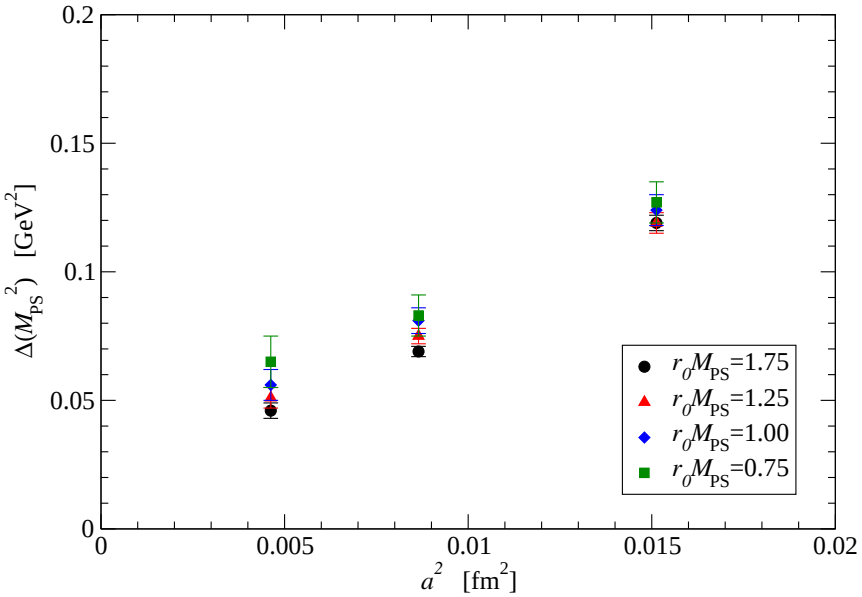


Fig. 12. The difference between charged and neutral squared pseudoscalar meson masses as a function of squared lattice spacing, for selected values of the charged meson mass. Plot taken from ref. [95]

.

An exploratory dynamical study with two light degenerate quark and two heavier non-degenerate quarks ($N_f = 2 + 1 + 1$) has been carried out in ref. [41], following the approach explained in sect. 2 with off-diagonal flavour splitting [38]. As we have already explained this approach has the big advantage of being well suited for dynamical simulation. Moreover it has been noted in [41] that with this formulation the masses in the kaon doublet (and D-meson doublet) are exactly degenerate. This follows from an exact symmetry of the lattice action defined in eq. (3.20). To understand how this works, we first write two interpolating fields for the kaon doublet in the physical basis (see sect. 5):

$$K^+(x) = \bar{u}(x)\gamma_5 s(x), \qquad K^0(x) = \bar{d}(x)\gamma_5 s(x). \tag{6.29}$$

Performing the rotations (3.2,3.5) we obtain in the twisted basis

$$K^+(x) = -\frac{i}{\sqrt{2}}\bar{u}(x)c(x) + \frac{1}{\sqrt{2}}\bar{u}(x)\gamma_5 s(x), \qquad K^0(x) = -\frac{1}{\sqrt{2}}\bar{d}(x)\gamma_5 c(x) - \frac{i}{\sqrt{2}}\bar{d}(x)s(x). \tag{6.30}$$

Both the action for degenerate u and d quarks in eq. (2.28) and for non degenerate s and c quarks in eq. (3.20) are symmetric under parity "times" flavour exchange $\mathcal{P}^1_F$ defined in eq. (2.38). Under this symmetry transformation the single flavoured

quarks transform as

$$\mathcal{P}_F^1\colon \begin{cases} u(x_0,\mathbf{x}) \to i\gamma_0 d(x_0,-\mathbf{x}) \\ d(x_0,\mathbf{x}) \to i\gamma_0 u(x_0,-\mathbf{x}) \\ c(x_0,\mathbf{x}) \to i\gamma_0 s(x_0,-\mathbf{x}) \\ s(x_0,\mathbf{x}) \to i\gamma_0 c(x_0,-\mathbf{x}) \end{cases}, \qquad \begin{cases} \bar{u}(x_0,\mathbf{x}) \to -i\bar{d}(x_0,-\mathbf{x})\gamma_0 \\ \bar{d}(x_0,\mathbf{x}) \to -i\bar{u}(x_0,-\mathbf{x})\gamma_0 \\ \bar{c}(x_0,\mathbf{x}) \to -i\bar{s}(x_0,-\mathbf{x})\gamma_0 \\ \bar{s}(x_0,\mathbf{x}) \to -i\bar{c}(x_0,-\mathbf{x})\gamma_0 \end{cases}. \tag{6.31}$$

The effect of this *exact* symmetry transformation is

$$K^+(x_0,\mathbf{x}) \to K^0(x_0,-\mathbf{x}), \qquad K^0(x_0,\mathbf{x}) \to K^+(x_0,-\mathbf{x}). \tag{6.32}$$

Hence the equality of the masses within kaon doublets follows. It is straightforward to repeat the same argument to show that also the D-doublet is mass degenerate.

6.4.3 Baryon splitting

In principle $\mathrm{O}(a^2)$ isospin breaking cutoff effects can appear also in baryon correlators. Here we concentrate on the spin-parity $(1/2)^\pm$ and $(3/2)^\pm$ baryons and we always consider Wtm with two degenerate quarks as specified by the action in eq. (2.28).

We write now the interpolating fields for the baryons in the *physical basis*

$$\mathscr{P} = \epsilon_{ABC}[u_A^T C^{-1}\gamma_5 d_B]u_C, \tag{6.33}$$
$$\mathscr{N} = \epsilon_{ABC}[d_A^T C^{-1}\gamma_5 u_B]d_C, \tag{6.34}$$
$$\Delta_k^{++} = \epsilon_{ABC}[u_A^T C^{-1}\gamma_k u_B]u_C, \tag{6.35}$$
$$\Delta_k^{+} = \frac{2}{\sqrt{3}}\epsilon_{ABC}[u_A^T C^{-1}\gamma_k d_B]u_C + \frac{1}{\sqrt{3}}\epsilon_{ABC}[u_A^T C^{-1}\gamma_k u_B]d_C, \tag{6.36}$$
$$\Delta_k^{0} = \frac{2}{\sqrt{3}}\epsilon_{ABC}[d_A^T C^{-1}\gamma_k u_B]d_C + \frac{1}{\sqrt{3}}\epsilon_{ABC}[d_A^T C^{-1}\gamma_k d_B]u_C, \tag{6.37}$$
$$\Delta_k^{-} = \epsilon_{ABC}[d_A^T C^{-1}\gamma_k d_B]d_C, \tag{6.38}$$

where C is the charge conjugation matrix defined in app. B. To get the corresponding interpolating fields in the *twisted basis* it is enough to apply the rotation in eq. (2.6) to the quark fields. In app. F, I show how this works with the proton field. Here I just want to prove that the proton and the neutron with Wtm are degenerate even at finite lattice spacing. This was shown in ref. [68] and here we give a slightly different argument based on the symmetries of the lattice action. In particular we know that parity "times" flavour exchange $\mathcal{P}_F^1$, defined in eq. (2.38) is a symmetry of Wtm. This symmetry is independent on the basis of choice, in fact also the action in the physical basis (5.3) is invariant under the $\mathcal{P}_F^1$ symmetry transformation. Applying

this symmetry to the baryon fields we obtain

$$\mathscr{P}(x_0, \mathbf{x}) \to -i\gamma_0 \mathscr{N}(x_0, -\mathbf{x}) \tag{6.39}$$

$$\Delta_k^{++}(x_0, \mathbf{x}) \to -i\gamma_0 \Delta_k^{-}(x_0, -\mathbf{x}) \tag{6.40}$$

$$\Delta_k^{+}(x_0, \mathbf{x}) \to -i\gamma_0 \Delta_k^{0}(x_0, -\mathbf{x}). \tag{6.41}$$

If we consider a baryon field $\mathscr{B}$ and the corresponding correlation function

$$a^3 \sum_{\mathbf{x}} \langle \mathscr{B}(x_0, \mathbf{x}) \bar{\mathscr{B}}(0, \mathbf{0}) \rangle, \tag{6.42}$$

we conclude that proton and neutron are degenerate as are Δ_k^{++} with Δ_k^{-} and Δ_k^{+} with Δ_k^{0}. There is on the other hand an $\mathrm{O}(a^2)$ splitting between Δ_k^{++} and Δ_k^{+}. This splitting it is also numerically simpler to study than the pion splitting since it does not require computation of disconnected diagrams. This was in fact noticed and studied in ref. [68] in the quenched model. Figs. 13 and 14 show the results for the splitting in physical units in the Δ channel, as obtained respectively from the "Wilson pion" definition of the critical mass and the "ω_A method". No significant difference is found between the two definitions of full twist for this observable. Based on the larger statistics of fig. 13 (1000 configurations rather than only 300), there is some evidence that $m_{\Delta^{++,-}} - m_{\Delta^{+,0}}$ decreases as $a \to 0$, as expected.

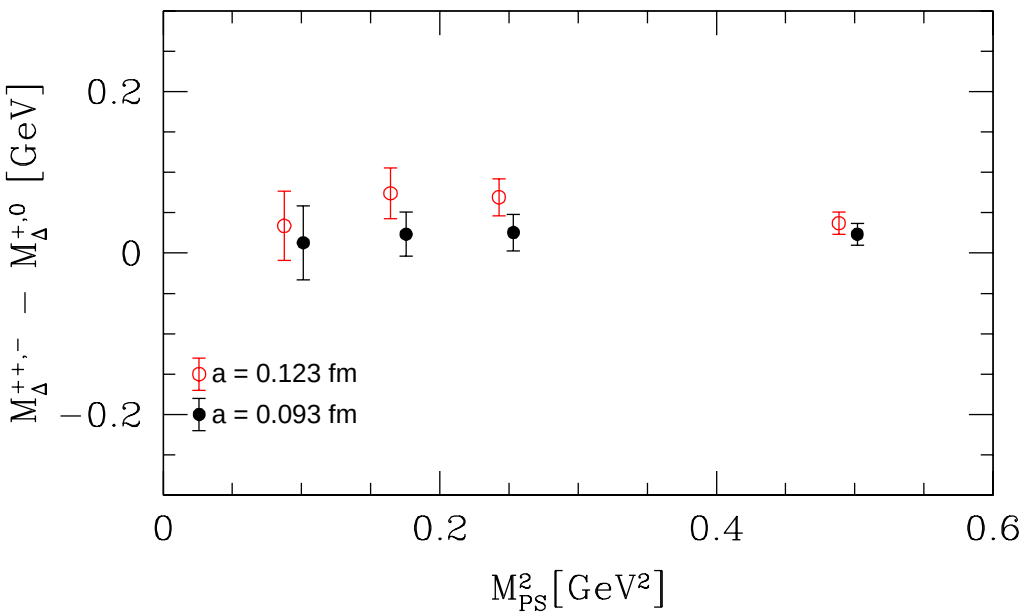


Fig. 13. Flavour splitting within the $\Delta(1232)$ multiplet as a function of the pseudoscalar meson mass squared, for two lattice spacings: $a = 0.123$ fm (○) and $a = 0.093$ fm (●). The critical mass was fixed using the "Wilson pion" method.

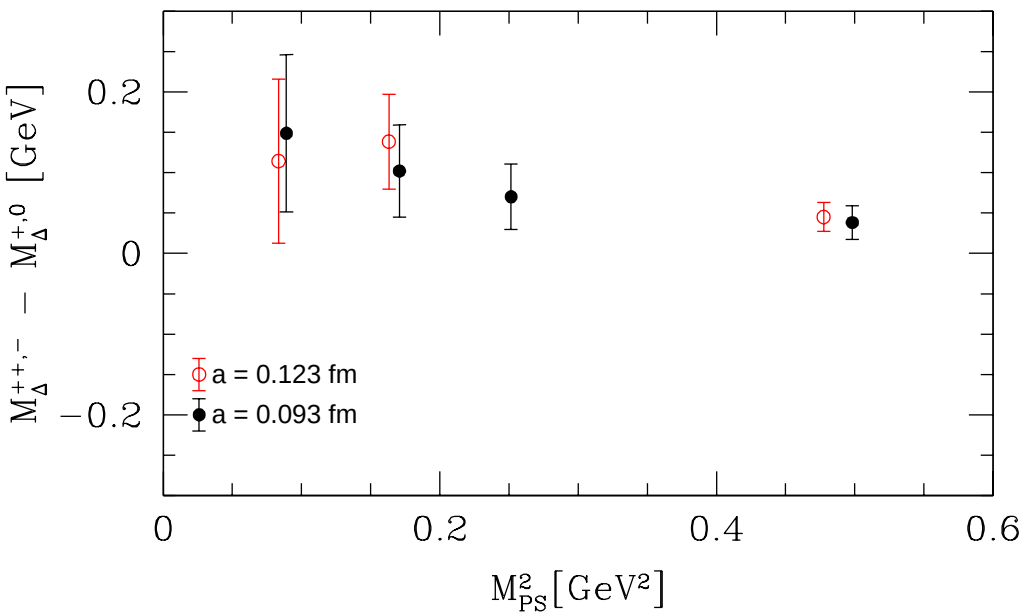


Fig. 14. Same as fig. (13) but with the critical mass fixed using the "ω_A method".

The extension of WχPT, with a twisted mass term, to include the baryons has been worked out in ref. [102]. In this work, beside showing how to include the baryons in the effective theory, several interesting results have been obtained. It has been confirmed automatic O(a) improvement at full twist for baryon masses, it has been discussed the splittings among the delta-resonances and a mass splitting formula has been given for a genric twist angle ω.

6.4.4 Conclusions

Isospin breaking cutoff effects are most probably the most delicate issue concerning Wtm. In the pseudoscalar sector they are similar in magnitude with the staggered taste violating cutoff effects, and they are even smaller if we include the disconnected diagrams in the pion sector. The possibility to use the OS action for the valence quarks partially mitigates this problem. The mixed action approach, while removing completely the isospin breaking at the valence level, cannot cure completely the problem. For physical quantities which involve pion scattering, isospin breaking cutoff effects are an issue which has to be further investigated. In the baryon sector isospin breaking cutoff effects seem to be under control. Moreover choosing as a lattice action for the heavy non-degenerate quarks the action proposed in [38] the splitting in the K and D sector is absent.

6.5 Phase structure of Wilson fermions

In the first part of this sect. 6, we have discussed the $O(a^2)$ isospin breaking cutoff effects. Now we want to analyze the impact of the $O(a^2)$ discretization errors the shape of the chiral phase diagram. The $O(a^2)$ chirally breaking cutoff effects change the form of the chiral phase transition. Thus the knowledge of the shape of the chiral phase diagram is an important prerequisite to perform large scale simulations with a given lattice action. In this section I show that both numerically and analytically there is strong evidence that Wilson type fermions show a peculiar phase diagram around the chiral point. The structure of such a phase diagram is due to lattice artifacts. We will see in sect. 8 that the approach to the chiral and continuum limit in numerical simulations shows a substantial slowing down in algorithmic performance, so in general a careful continuum limit and chiral extrapolation is required in order to compare lattice results with experimental measurements. The knowledge of the position of the phase transition point as a function of the quark mass and the lattice spacing, becomes then very important, given also the fact that it is not clear whether HMC-like algorithms can correctly sample the configuration space in such extreme situations. In particular the shape of the phase structure is such that there is a minimal pion mass that can be simulated at fixed lattice spacing. This bound depends on the details of the Wilson-like action used in the simulations (e.g. on the gauge action). Lattice simulations are performed in a finite volume and strictly speaking there are no phase transitions in a finite box, but if the lattice size is large enough, the shadow of the would-be phase transition could still be visible in the numerical simulations.

6.5.1 $W\chi PT$ analysis

Before going into the study of the phase diagram of Wilson-like fermions let us recall which is the situation in continuum QCD. In the continuum chiral symmetry is spontaneously broken in the massless limit, and the order parameter of such a transition is the chiral condensate. The structure of the phase diagram is thus simply: a singular point at the origin of the "mass plane" where we plot the untwisted quark mass along the horizontal axis and the twisted mass along the vertical axis (see fig. 15). The aim of this section is to understand how this picture is modified by the inclusion of lattice artifacts in the chiral Lagrangian. We have already discussed in sect. 4.3.2 the construction of the chiral Lagrangian including lattice spacing effects. In particular our starting point was the power counting scheme specified in eq. (4.67). We have seen in sect. 4.3.2 that at LO the inclusion of $O(a)$ lattice artifacts can be fully reabsorbed in a shifted quark mass m', defined in eq. (4.71). We can then immediately conclude that if we are in the power counting scheme given by eq. (4.67) the phase structure is continuum like. To start to be sensitive to

the modifications of the phase structure in presence of lattice artifacts we have to further lower the quark masses at fixed lattice spacing. In particular the appropriate power counting is given

$$1 \gg m', \mu_{\rm R}, p^2, a^2 \gg \dots \tag{6.43}$$

This region of quark masses is usually called the Aoki region because it is the region where a possible Aoki phase appears [12]. The Aoki phase, as we will see below, is characterized by a region in the bare parameters space where parity and flavour are spontaneously broken.

Since we are changing the power counting scheme, the careful reader could wonder if this does not imply a breakdown of the expansion. The reason why this is not the case is that there is a rearrangement in the ordering of the coefficients of the chiral Lagrangian. It is possible to show [78] that the neglected terms of the expansion are at most of order $\sim a^3$, and thus suppressed by one power of a. Loop corrections are also suppressed, since they are quadratic in m' and $\mu_{\rm R}$ (up to logarithms) and thus $\sim a^4$. The reordering of the expansion is possible only because the leading order discretization error has exactly the form of a mass term and so can be completely absorbed into m', to all orders in the chiral expansion [78].

Upon neglecting the derivative interaction terms, as we are interested in the vacuum state, the potential of the effective chiral Lagrangian at LO [55, 83, 96, 103] is given by

$$V_\chi = -\frac{c_1}{4}\langle \Sigma + \Sigma^\dagger \rangle + \frac{c_2}{16}\langle \Sigma + \Sigma^\dagger \rangle^2 + \frac{c_3}{4}\langle i(\Sigma - \Sigma^\dagger)\tau_3 \rangle \tag{6.44}$$

where the explicit forms of the coefficients, and their sizes in our power-counting scheme, are

$$\begin{aligned} c_1 &= 2B_0 f^2 m' \sim m', \\ c_2 &= -f^2 w' a^2 \sim a^2, \\ c_3 &= 2B_0 f^2 \mu_{\rm R} \sim \mu_{\rm R}, \ . \end{aligned} \tag{6.45}$$

All the c_i coefficients are independent at non-zero lattice spacing and the only extra term introduced by the twisted mass is the one proportional to c_3.

In the Aoki region the coefficient c_2 is of the same size as the coefficients $c_{1,3}$; all are of $O(a^2)$. This implies a competition of the mass terms and the O(a^2) term in the shape of the potential that causes a non-trivial vacuum structure. Minimizing the potential (6.44) gives rise to two possible scenarios [78, 83, 96, 103] for the phase diagram of Wilson-like fermions:

- the Aoki scenario [12];
- the Sharpe-Singleton scenario [78].

Note that *both* m' and $\mu_{\rm R}$ must be of $O(a^2)$ in order for such competition to occur; if either m' or $\mu_{\rm R}$ is of $O(a)$ then one is in the continuum-like region. I would like to remark that the presence of two possible phase structures was foreseen by Creutz [104].

The order parameter of the continuum chiral phase transition is the chiral condensate. The condensate in WχPT is determined by the minima of the potential energy (6.44). We parametrize the chiral field in the standard way: $\Sigma = \Sigma_0 + i\Sigma_a \cdot \tau^a$ with real Σ_0 and Σ_a satisfying $\Sigma_0 \cdot \Sigma_0 + \Sigma_a \cdot \Sigma_a = 1$, so that $\Sigma_0,\, \Sigma_a \in [-1, 1]$. Similarly, the condensate (the value of Σ at the minimum of the potential) is written $\Sigma_0^{(m)} = \Sigma_0^{(m)} + i\Sigma_a^{(m)} \cdot \tau^a$. In the Aoki region the potential is then

$$V_\chi = -c_1\Sigma_0 - c_3\Sigma_3 + c_2\Sigma_0^2\,. \tag{6.46}$$

We have now to compute the values of $\Sigma_0^{(m)}$ and $\Sigma_3^{(m)}$. We will not enter in the details of the computations that are nevertheless rather simple. One finds that there two possible solutions depending on the sign of c_2 (or w'). Thus it is the sign of c_2 (or w') that determines the possible scenario for the chiral phase structure of Wilson-like fermions. We summarize here the results illustrating them with plots [96]. For convenience we define the following rescaled mass variables

$$\mathfrak{m} = \frac{c_1}{|c_2|} = \frac{2B_0 m'}{a^2|w'|} \sim m'/a^2 \tag{6.47}$$

$$\mathfrak{n} = \frac{c_3}{|c_2|} = \frac{2B_0 \mu_{\rm R}}{a^2|w'|} \sim \mu_{\rm R}/a^2\,. \tag{6.48}$$

They are of O(1) in the region of interest.

In fig. 15 I plot the lines corresponding to a first order phase transition which have second order phase transitions end points, where the x-axis is $\mathfrak{m}$ and the y-axis is $\mathfrak{n}$.

I first discuss the structure of the phase diagram for c_2 positive or negative and then I will describe the physics one finds in the two situations.

In the left panel of fig. 15 the Aoki scenario that appears if $c_2 > 0$ ($w' < 0$) is depicted. In this scenario along the Wilson axis $\mathfrak{m}$ there is a region (indicated by the thick line) where parity and flavour are spontaneously broken: this is the Aoki phase [12]. At the endpoints of this line the three pions are massless. Inside the Aoki phase the charged pions stay massless while the neutral one becomes massive. A non-zero value of the twisted mass washes out the Aoki phase introducing an explicit breaking of flavour and parity symmetry.

In the right panel of fig. 15 the Sharpe-Singleton scenario that appears if $c_2 < 0$ ($w' > 0$) is depicted. In this scenario the first order phase transition line extends

into the twisted direction. The transition ends with a second order phase transition point, where the neutral pion mass vanishes.

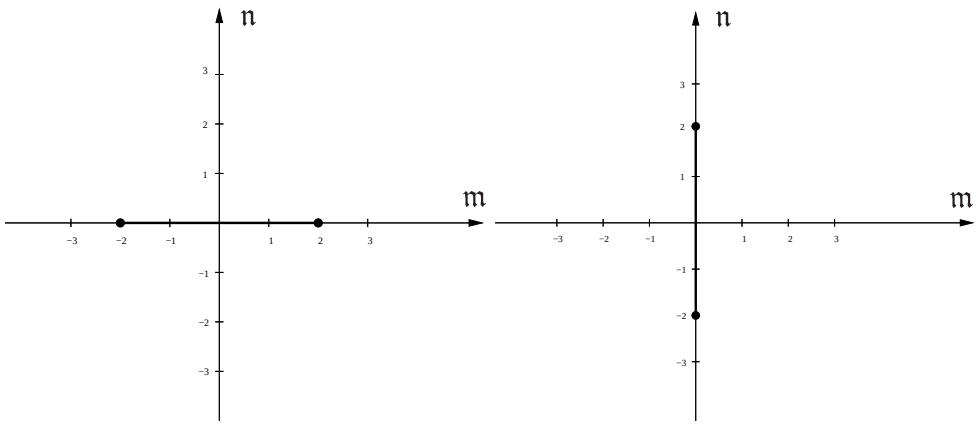


Fig. 15. Left panel: the phase diagram of Wilson diagram according to Wχ PT for $c_2 > 0$. Right panel: as in the left panel but for $c_2 < 0$. The x-axis is proportional to m'/a^2 and the y-axis to $\mu_{\rm R}/a^2$ (6.47,6.48).

We go now to study the mass dependence of the condensate and of the pion masses inside the Aoki region.

We begin with results for $c_2 > 0$. Fig. 16 shows the behaviour of the identity component of the condensate, $\Sigma_0^{(m)} = \langle \Sigma^{(m)} \rangle / 2$, for $\mathfrak{n} = 0$, 1, 2 and 3 as a function of $\mathfrak{m}$. The corresponding pion masses are shown in fig. 17. In the untwisted theory ($\mathfrak{n} = 0$) there are second order transitions at $m' = \pm \frac{a^2 |w'|}{B_0}$, as shown by the discontinuity in the derivatives respect to $\mathfrak{m}$ in $\Sigma_0^{(m)}$ and the vanishing of the pion masses. In the Aoki phase, with $\Sigma_3^{(m)} \neq 0$, the $SU_{\rm V}(2)$ vector flavour symmetry is spontaneously broken into $U_{\rm V}(1)_3$, and correspondingly there are two Goldstone bosons between these second-order points. Once $\mathfrak{n}$ is non-vanishing, however, the transition is smoothed out into a crossover, and the pion masses are always non-zero. Flavour is broken for

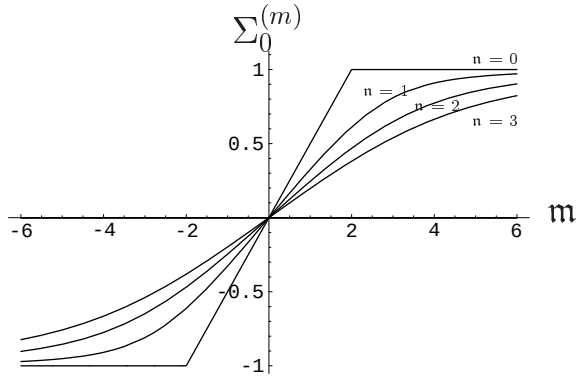
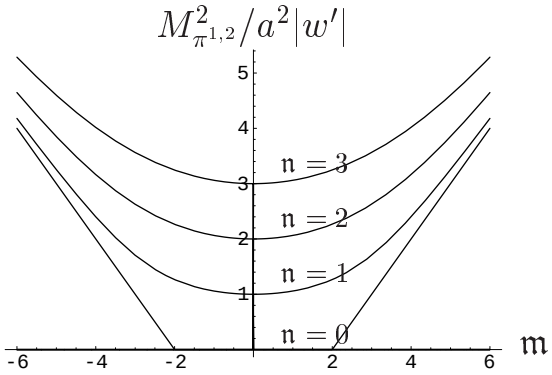
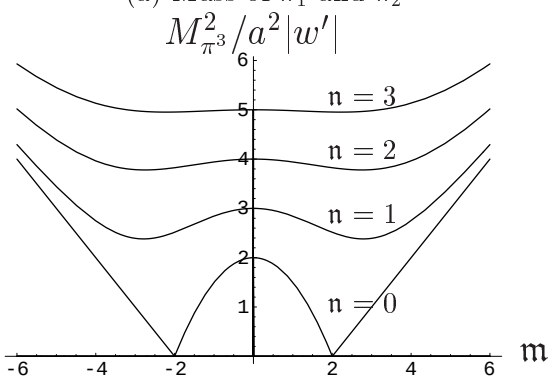


Fig. 16. The global minimum of the potential, $\Sigma_0^{(m)}$, as a function of $\mathfrak{m}$, for $c_2 > 0$ and $\mathfrak{n} = 0$, 1, 2, 3.



(a) Mass of π_1 and π_2



(b) Mass of π_3

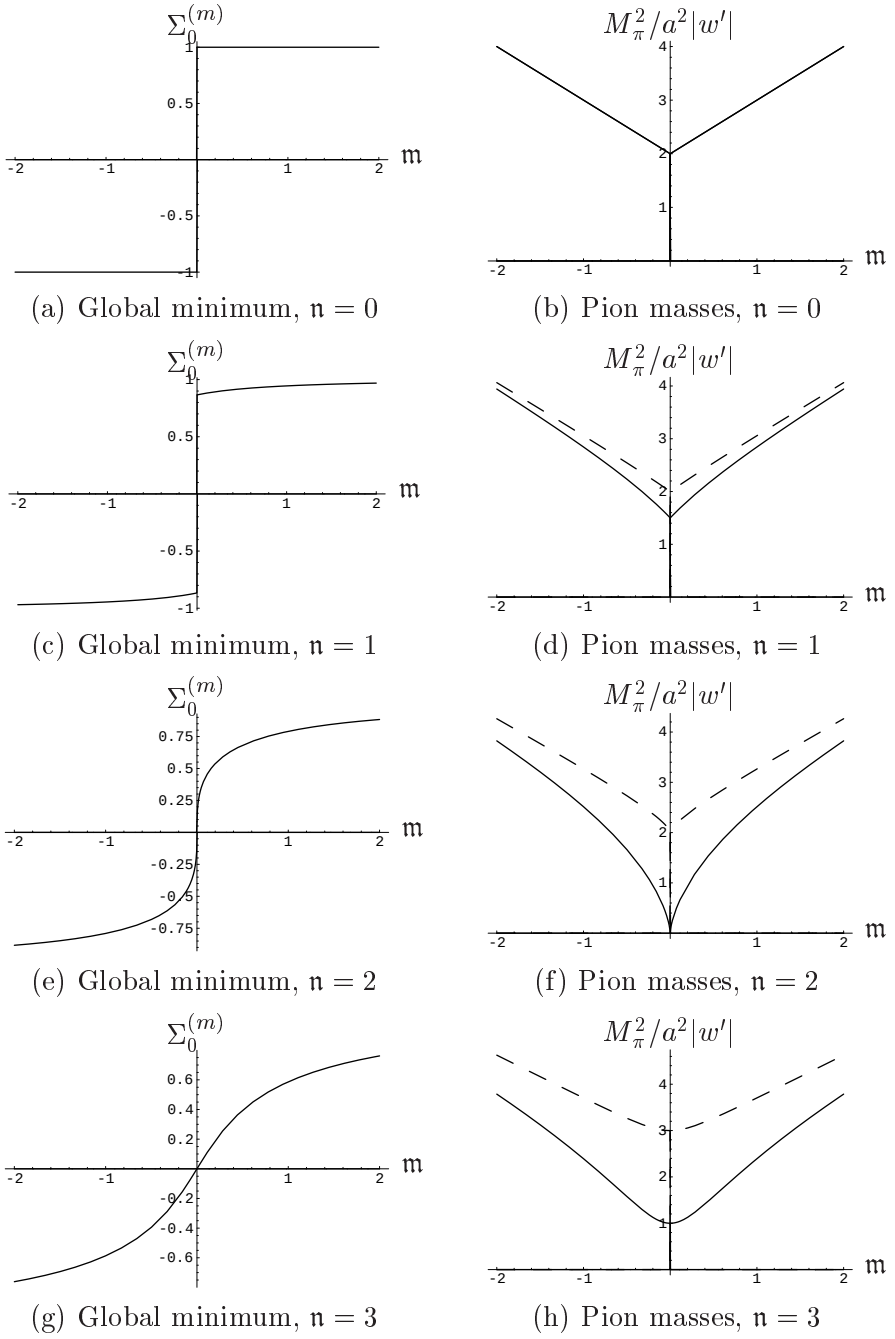
Fig. 17. Mass of the pions as a function of $\mathfrak{m}$, for $c_2 > 0$ and $\mathfrak{n} = 0$, 1, 2, 3.

all $\mathfrak{m}$, with the charged pions lighter than the neutral pion by $O(a^2)$, as given by eq. (6.25). For the special case of $\mathfrak{m} = 0$ (full twist), $\Sigma_0^{(m)}$ vanishes and $(\Sigma_3^{(m)})^2 = 1$, so the mass-squared splitting is $2a^2|w'|$ for all $\mathfrak{n}$ (which becomes a difference of 2 in the units in the plots).

If we keep $-2 \leq \mathfrak{m} \leq 2$ fixed, and we lower $\mathfrak{n}$, it is possible to pass through the Aoki phase. When we change the sign of twisted mass, i.e. passing through $\mathfrak{n} = 0$, there is a first-order phase transition, since $\Sigma_3^{(m)}$ jumps from $+\sqrt{1-(\Sigma_0^{(m)})^2} = \sqrt{1-\mathfrak{m}^2/4}$ to $-\sqrt{1-(\Sigma_0^{(m)})^2} = -\sqrt{1-\mathfrak{m}^2/4}$.

We now consider the case where c_2 is negative. Fig. 18 shows $\Sigma_0^{(m)}$ and the pion masses as a function of $\mathfrak{m}$ for fixed values of $\mathfrak{n}$. Fig. 18(a) and fig. 18(b) show the results for $\mu_{\mathrm{R}} = 0$. The condensate jumps from $\Sigma_0 = 1$ (and thus $\Sigma_0^{(m)} = 1$, $\Sigma_a^{(m)} = 0$) for $\mathfrak{m} > 0$ to $\Sigma_0 = -1$ (and thus $\Sigma_0^{(m)} = -1$, $\Sigma_a^{(m)} = 0$) for $\mathfrak{m} < 0$. This is a first order transition without flavour breaking, so all pions remain massive and degenerate.

The rest of fig. 18 shows what happens at non-zero twisted mass. The effect of μ_{R} is to twist the condensate, so that there is a non-zero τ_3 component $\Sigma_3^{(m)}$. There is,



(a) Global minimum, $\mathfrak{n} = 0$ (b) Pion masses, $\mathfrak{n} = 0$

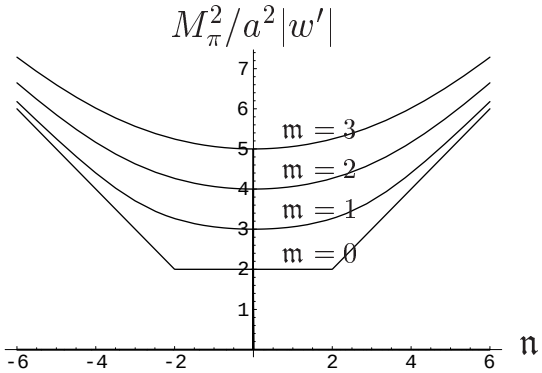
(c) Global minimum, $\mathfrak{n} = 1$ (d) Pion masses, $\mathfrak{n} = 1$

(e) Global minimum, $\mathfrak{n} = 2$ (f) Pion masses, $\mathfrak{n} = 2$

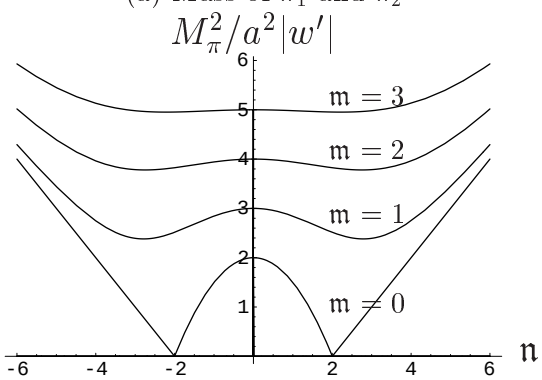
(g) Global minimum, $\mathfrak{n} = 3$ (h) Pion masses, $\mathfrak{n} = 3$

Fig. 18. Global minimum $\Sigma_0^{(m)}$ and pion masses as a function of $\mathfrak{m}$, for $c_2 < 0$ and $\mathfrak{n} = 0$, 1, 2, 3. The dashed lines are for $\pi_{1,2}$ and the solid lines are for π_3.

however, still a first order transition at which $\Sigma_3^{(m)}$ flips sign between $\pm(1 - \mathfrak{n}/2)$ (assuming $\mathfrak{n} > 0$). The neutral pion is now lighter than the charged pions due to explicit flavour breaking. The neutral pion has a mass $M_{\pi_3}^2 = 2a^2|w'|(1 - \mathfrak{n}/2)^2$ at the transition, while, as noted above, the charged pions have a $\mathfrak{n}$ independent mass given by $m_{\pi_{1,2}}^2 = 2a^2|w'|$. The transition weakens as $|\mathfrak{n}|$ increases, and ends with a



(a) Mass of π_1 and π_2



(b) Mass of π_3

Fig. 19. Mass of the pions as a function of $\mathfrak{n}$, for $c_2 < 0$ and $\mathfrak{m} = 0$, 1, 2, 3.

second order transition point at $\mathfrak{n} = \pm 2$, at which the neutral pion is massless [see Fig. 18(f))]. For larger $\mathfrak{n}$ the transition is smoothed out. Note that, once away from the transition, for $\mathfrak{m} = 0$ the mass-squared splitting between charged and neutral pions is still $2a^2|w'|$ and independent from $\mathfrak{n}$.

These plots illustrate the general fact that the $c_2 < 0$ case can be obtained from that with $c_2 > 0$ by a $\pi/2$ rotation and appropriate redefinitions. Indeed, the results for $c_2 > 0$ can alternatively be viewed as the plots for $c_2 < 0$ at fixed $\mathfrak{m}$ with $\mathfrak{n}$ varying, and *vice versa*, with the exception of the charged pion masses, which differ by a constant offset of $2|c_2|/f^2$. To illustrate this latter point I plot, in fig. 19, the pion masses for $c_2 < 0$ as a function of $\mathfrak{n}$ for fixed values of $\mathfrak{m}$. Comparing to fig. 17, we see the equality of the neutral pion masses and the constant offset in the charged pion masses.

6.5.2 Numerical results

The analysis carried out with WχPT is very predictive but cannot choose between the two possible shapes of the potential. The occurrence of one of the two scenarios depends on the sign of the coefficient c_2 proportional to the $O(a^2)$ terms of the chiral

Lagrangian, and this coefficient c_2, similarly to the other LEC, it is not determined by chiral symmetry, but it depends on the details of the lattice action one is using, like the gauge action, the presence in the lattice action of the clover term and of course it depends on the value of the bare gauge coupling, i.e. of the lattice spacing.

The lattice spacing dependence of the phase structure can be studied in detail using lower dimensional models, allowing a better analytical control over the computations. An analysis with Wilson fermions of the two dimensional Gross-Neveau model [105] indicates that indeed both the scenarios describe the phase structure of Wilson fermions depending on the value of the couplings of the model. The analysis shows that at strong coupling there is an Aoki phase while at weak coupling the Sharpe-Singleton scenario sets in. This analysis has been recently extended for the twisted mass case [106], indicating even more complicated structures, like a coexistence of the two scenarios for certain values of the bare couplings.

In QCD the situation is more involved. The prediction of the existence of an Aoki-phase was made years before the analysis of WχPT [12, 107, 108]. The existence of a region of bare parameters where parity and flavour were spontaneously broken was a possible mechanism to generate a massless pion at finite lattice spacing. Quenched studies [109–111] found evidence of such a phase structure. Recently a quenched computation [94] of the charged and neutral pseudoscalar masses using Wtm has shown that the charged pion is lighter than the neutral, indicating that in the quenched case we are in an Aoki scenario.

On the other hand it is interesting to revisit some old controversial results about the chiral phase structure of Wilson fermions, using the standard Wilson gauge action (2.26). In [112, 113] from a finite temperature study there was an indication of difficulties in observing a phase with spontaneous breaking of flavour and parity symmetry (Aoki phase) at $\beta > 4.8$. In [114] the MILC collaboration found a surprising bulk first order phase transition at $\beta \simeq 4.8$. In a recent investigation [115] of the Aoki phase for values of the coupling $\beta < 5$ the authors confirm evidence for an Aoki phase but only for values $\beta < 4.6$. For values of $\beta > 5$ with Wilson plaquette gauge action a systematic investigation was missing.

This gap has been filled in a set of publications that have thoroughly investigated the chiral phase structure of Wilson-like fermions. In [116] the first study of Wtm with $N_{\rm f} = 2$ dynamical fermions was performed and rather surprising results were found: the existence of the Sharpe-Singleton scenario.

The action used in this study is Wilson gauge action combined with Wilson fermions with and without twisted mass. In particular at a lattice spacing of $a \approx 0.16$ fm, strong evidence of a first order phase transition was found for a rather large range of values of twisted masses going from zero twisted mass to $\mu_{\rm q} \simeq 100$ MeV. This study reveals also that the phase transition tends to disappear on increasing the value of

μ_q, it persists for $\mu_q = 0$ and it is volume independent.

This study was extended in [117]. In fig. 20 I show scans of the average plaquette and $m_{\rm PCAC}$ at fixed twisted mass (with μ_q roughly fixed in physical units) for three decreasing lattice spacings (at increasing β values). The plaquette and $m_{\rm PCAC}$ both have a discontinuity, and show hysteresis. Both effects decrease as one approaches the continuum limit, qualitatively consistent with expectations. The fact that $m_{\rm PCAC}$ has a minimum away from zero is a manifestation of the non-zero minimum in the pion masses.

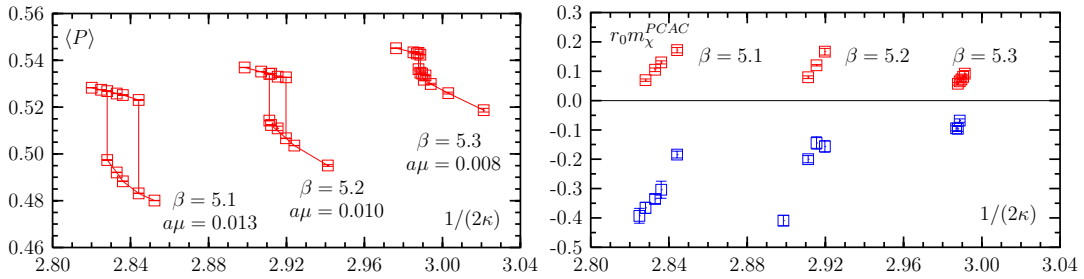


Fig. 20. Average plaquette and $m_{\rm PCAC}$ plotted vs. $(2\kappa)^{-1} = m_0 + 4$ for fixed μ_q [117].

Our present understanding of the lattice QCD phase diagram with Wilson gauge action and Wilson-like fermions can be summarized as follows. For values of the lattice spacing much coarser than $a = 0.15$ fm, there is an Aoki phase [12, 115, 118]. For smaller values of the lattice spacing, a first order phase transition appears (Sharpe-Singleton scenario) [84,116,117,119] that separates the positive quark mass from the negative quark mass phase, and extends into the twisted direction. This first order phase transition is reminiscent of the continuum phase transition when the quark mass is changed from positive to negative values with the corresponding jump of the scalar condensate which is the order parameter of spontaneous chiral symmetry breaking. The generic phase structure of lattice QCD is illustrated in fig. 21 and discussed in refs. [84, 116, 119].

6.5.3 The gauge action

In the Sharpe-Singleton scenario, the pseudoscalar mass $m_{\rm PS}$ cannot be made arbitrarily small. When lowering the quark mass from the twisted direction there is a minimal pion mass accessible with numerical simulations given directly by the extension of the first order phase transition line, even if the twisted mass provides a sharp infrared cutoff in the sampling performed by the simulation algorithm.

An important result of WχPT is that both the size of the phase boundaries and the isospin splitting for pions are determined by the same parameter, w'. It thus makes sense to try and tune the gauge and fermion actions to reduce $|w'|$. Note that this

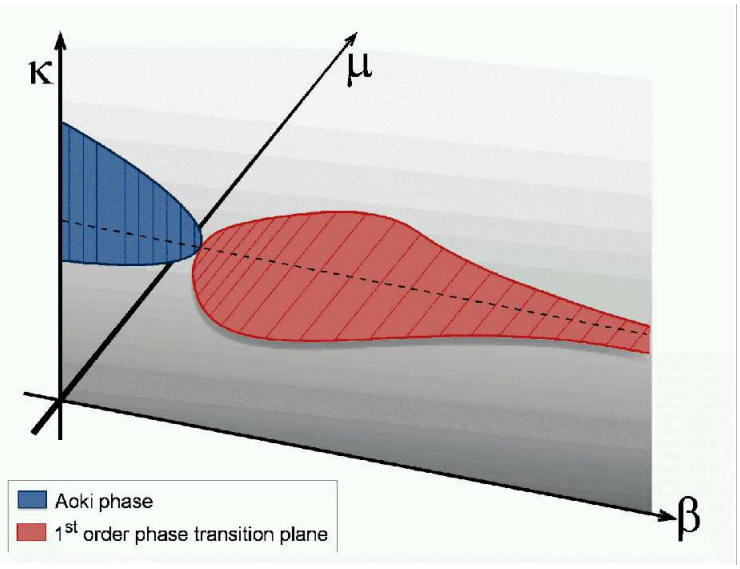


Fig. 21. Current knowledge of the Wilson lattice QCD phase diagram as function of the inverse gauge coupling $\beta \propto 1/g^2$, the hopping parameter $\kappa = (8+2am_0)^{-1}$ and the twisted mass parameter $\mu_{\rm q}$.

tuning is not the same as a systematic improvement program, but it is nevertheless very important.

In [117] the lattice spacing dependence of the first order phase transition with Wilson gauge action has been studied, taking, as a measure of its strength, the gap between the two phases in the plaquette expectation value and in the PCAC quark mass. The qualitative estimate for the lattice spacing, where a minimal pion mass $m_\pi \simeq 300$ MeV could be reached without being affected by the first order first transition is 0.07-0.1 fm.

It is suggestive to interpret, at the microscopic level, the occurrence of the Sharpe-Singleton scenario with a massive rearrangement of the small eigenvalues of the Wilson-Dirac around the first order phase transition line. This rearrangement could be suppressed by the use of a renormalization group improved or $O(a^2)$ improved gauge action, and indeed results from [120] indicate that metastabilities in the average plaquette observed for $N_{\rm f} = 3$ dynamical Wilson fermions with a clover term can be suppressed replacing the Wilson gauge action with the Iwasaki action [121].

The dependence of the phase diagram on the gauge action used and on the lattice spacing has been studied in a set of papers [84, 116, 117, 119] (see also [122] for a detailed summary of these results). The gauge actions studied so far can be parametrized by

$$S_{\rm G} = \frac{\beta}{6}\Big[b_0 \sum_{x;\mu\neq\nu} {\rm tr}(1 - P^{1\times 1}(x;\mu,\nu)) + b_1 {\rm tr}(1 - P^{1\times 2}(x;\mu,\nu))\Big] \qquad (6.49)$$

with the normalization condition $b_0 = 1 - 8b_1$. In particular three gauge actions have been investigated:

- Wilson action [1] $\Rightarrow b_1 = 0$
- tree-level Symanzik action [123] $\Rightarrow b_1 = -\frac{1}{12}$
- DBW2 action [124] $\Rightarrow b_1 = -1.4088$

The result of these studies is summarized in fig. 22 which shows that the discontinuities in the plaquette are significantly reduced going from the Wilson to the DBW2 gauge action.

By varying the coupling b_1 which multiplies the rectangular plaquette term, one can interpolate between various actions and this allows to understand in more detail the properties of the phase structure, in particular how the strength of the transition depends on the additional term and how this influences the approach to the continuum limit.

That even a small value of b_1 can already have a large impact on the phase structure is illustrated in fig. 22 which shows the average plaquette value as a function of the hopping parameter κ for three different actions, i.e. values of b_1, namely $b_1 = 0$ (Wilson), $b_1 = -1/12$ (tlSym) and $b_1 = -1.4088$ (DBW2). As one moves κ from

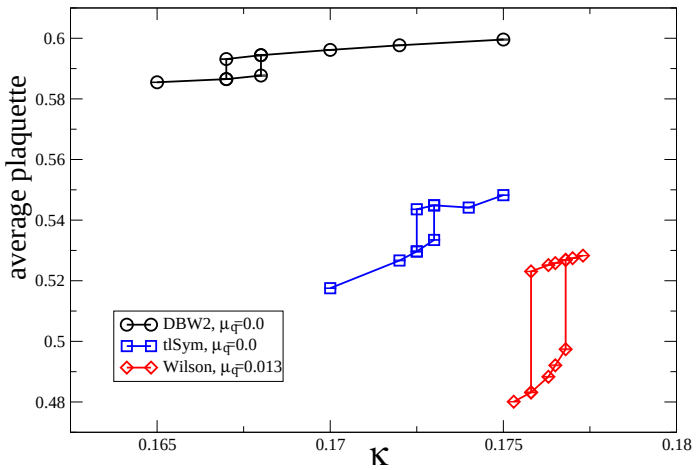


Fig. 22. Hysteresis of the average plaquette value as κ is moved across the critical point, for Wilson, tlSym and DBW2 gauge action at $a \sim 0.17$ fm.

the negative or positive side across the critical point, where the PCAC quark mass vanishes, a hysteresis in the average plaquette value develops whose size and width are indicators of the strength of the phase transition. Both the width and the size of the gap in the plaquette value decreases considerably as we switch on b_1 to $b_1 = -1/12$ (tlSym action). Decreasing b_1 further down to $b_1 = -1.4088$ (DBW2 action) still seems to reduce the size of the gap, but the effect is surprisingly small despite

the large change in b_1.[19] The results in fig. 22 are for a lattice spacing $a \sim 0.17$ fm that is roughly the same for all three actions. I remark also that the strength of the first order phase transition weakens rapidly when the lattice spacing is made finer. This is illustrated in the left plot of fig. 20 for the case of the Wilson plaquette gauge action.

A satisfactory setup for dynamical simulations with, say, $N_f = 2$ flavours of quarks would be to reach pion masses of about $250-300$ MeV and a box size of $L > 2$ fm. At the same time, one should stay at full twist to realize automatic $\mathrm{O}(a)$ improvement. From all the results presented here it is conceivable that for the tlSym action this can be achieved with a reasonable computer time at $a \simeq 0.1$ fm on $L/a = 24$ lattices. Although for the DBW2 action the situation might be somewhat better, the advantages of the tlSym action, such as good convergence of perturbation theory and not big scaling violations as found in [125] for the DBW2 gauge action, suggests the tlSym gauge action as the action of choice.

Of course other options could be advocated like sticking to the Wilson gauge action but simulating maybe at an even smaller lattice spacing, or modifying some parts of the fermionic action like the form of the covariant derivatives or by adding the clover term. In [71] it has been found that using the clover improved fermion action reduces the pion isospin splitting and thus w'. This result cannot be considered however conclusive for two reasons: the disconnected diagrams were neglected in the computation of the neutral pion; it was a quenched study. We have seen that these are critical issues because going from quenched to unquenched simulations and/or including the disconnected diagrams can have dramatic impacts in the phase diagram like even changing the sign of w', i.e. greatly affecting the neutral pion mass.

[19] In fact, the reductions are greater than appears, as the results with the Wilson action are for $\mu_{\mathrm{q}} \neq 0$, where the transition is weaker than for $\mu_{\mathrm{q}} = 0$, which is the value used for the other actions.

7 Renormalization and weak matrix elements

In the previous sections we have extensively discussed the issue of the continuum limit and we have analyzed cutoff effects of order a and a^2 with Wtm.

Renormalization is necessary in order to perform the continuum limit and correctly evaluate hadronic matrix elements. Here we will not discuss the way how the renormalization is performed but only the mixing patterns of relevant physical quantities according to the lattice action used, i.e. according to the way the theory is regularized. Throughout the section we will assume that a mass independent renormalization scheme has been used, and that the scheme allows for a non-perturbative renormalization. Examples of such schemes are the so called RI-MOM scheme [126], and the Schrödinger functional (SF) [50, 51].

Whatever is the chosen strategy, the renormalization is a difficult problem, that becomes even more difficult if one considers four-quark operators which appear in the effective weak Hamiltonian. The details of the renormalization patterns strongly depend on the symmetries preserved by the regularization adopted, i.e. on the lattice action. Regularizations which preserve chiral symmetry are clearly advantageous [127–129], and are increasingly used despite their high computational costs [63]. If computationally cheaper quarks of the Wilson type are used instead, the operator renormalization is complicated, mainly due to the presence of power divergences [35, 130] and/or mixings induced by the explicit chiral symmetry violation. It is then more than welcome to make use of the possibility to ease the renormalization pattern of relevant physical quantities using Wilson-like quarks.

In this section I will give two examples of how Wtm can be used to reach this goal: the pseudoscalar decay constant and B_K. This result can be obtained using the relative freedom of choosing the twist angle depending on the flavour of the quark field appearing in the four-fermion operators. This freedom has been used in different ways in [39, 98] leading to milder renormalization patterns for the four-fermion operators relevant for the $\Delta I = 1/2$ rule. The basic ideas on how to achieve these simplifications can be understood in an easier way by analyzing in detail the renormalization of B_K. This is presented in sect. 7.2. A detailed treatment of the $\Delta I = 1/2$ rule goes beyond the scope of this report. We thus refer to the original papers [39,98] and references therein for a detailed analysis on this particular process.

7.1 Decay constants

The determination of the Cabibbo-Kobayashi-Maskawa (CKM) matrix elements is of phenomenological and theoretical interest and to test the unitarity of the CKM

matrix, it is crucial to have a precise determination of the matrix element $|V_{us}|$ that parametrizes the coupling of the $u \to s$ transition in the Standard Model (SM).

Lattice QCD computations can address this issue determining in a very precise way the decay constants of the pion and the kaon.

In fact the knowledge from first principles of f_K/f_π allows for an accurate determination of $|V_{us}|/|V_{ud}|$ from the ratio of leptonic kaon decay rates [131]:

$$\frac{\Gamma(K \to \mu\bar{\nu}_\mu(\gamma))}{\Gamma(\pi \to \mu\bar{\nu}_\mu(\gamma))} = K\frac{|V_{us}|^2 f_K^2 m_K \left(1-\frac{m_\mu^2}{m_K^2}\right)^2}{|V_{ud}|^2 f_\pi^2 m_\pi \left(1-\frac{m_\mu^2}{m_\pi^2}\right)^2}, \tag{7.1}$$

where the prefactor K on the r.h.s. takes into account radiative corrections. By combining the experimental result $\Gamma(K \to \mu\bar{\nu}_\mu(\gamma))/\Gamma(\pi \to \mu\bar{\nu}_\mu(\gamma))$ with the Lattice QCD determination of f_K/f_π and the experimental value of $|V_{ud}|$ one obtains $|V_{us}|$.

At the moment, the lattice errors dominate the uncertainty in the determination of $|V_{us}|$, thus it is important to have available a lattice action that can minimize possible sources of systematic uncertainty.

With Wtm it is possible to determine the pseudoscalar decay constant without any computation of renormalization factors and without the knowledge of any improvement coefficient, still with only $\mathrm{O}(a^2)$ cutoff effects. It is only necessary to correctly tune the untwisted bare quark mass to full twist as extensively detailed in sec. 4.

Due to the exact flavour symmetry of massless Wilson quarks, the situation with the vector Ward identity is the same as with Ginsparg-Wilson fermions, i.e. the classical PCVC relation (2.19) holds exactly on the lattice

$$\partial_\mu^* \langle \widetilde{V}_\mu^a(x) O(0)\rangle = -2\mu_\mathrm{q}\epsilon^{3ab}\langle P^b(x)O(0)\rangle \tag{7.2}$$

(where ∂_μ^* is the lattice backward derivative) with the point-split vector current

$$\widetilde{V}_\mu^a(x) = \frac{1}{2}\Big\{\overline{\chi}(x)(\gamma_\mu - 1)\frac{\tau^a}{2}U(x,\mu)\chi(x+a\hat{\mu}) + \overline{\chi}(x+a\hat{\mu})(\gamma_\mu+1)\frac{\tau^a}{2}U(x,\mu)^{-1}\chi(x)\Big\}, \tag{7.3}$$

and the local pseudoscalar density. This implies that the multiplicative renormalization constants of composite fields which belong to the same isospin multiplet must be identical in order to respect the vector Ward identities. An example is the renormalized pseudoscalar density which has the structure

$$P_\mathrm{R}^a = Z_\mathrm{P}(P^a + \delta^{a3}\frac{c_\mathrm{P}}{a^3}). \tag{7.4}$$

The mixing with the identity operator appears because standard parity is not a symmetry of the massive lattice theory, but while $P^{1,2}$ are still protected by the

symmetries $\mathcal{P}_F^{1,2}$ defined in eqs. (2.38), P^3 is not. The vector Ward identity (7.2) here implies that $Z_{\rm P}$ is the same for all flavour components, and

$$Z_{\rm P} = \frac{1}{Z_\mu}. \tag{7.5}$$

Moreover since standard parity combined with a change of the sign of the twisted mass $\widetilde{\mathcal{P}}$ defined in eq. (2.39) is a symmetry of the lattice action, the mixing pattern of P^3 is actually only with a quadratically divergent term $\frac{\mu_{\rm q}}{a^2}$ similarly to what happens with overlap fermions.

The existence of the point-split vector current can be used as a tool to determine the finite renormalization constant $Z_{\rm V}$ that normalizes the local vector current. One possibility would be to determine $Z_{\rm V}$ through

$$Z_{\rm V} = \lim_{\mu_{\rm q}\to 0} \frac{\langle \widetilde{V}^a_\mu(x) O(0)\rangle}{\langle V^a_\mu(x) O(0)\rangle} \tag{7.6}$$

with the local vector current defined in eq. (2.10). This method requires the computation of a correlation function involving the point-split current. This can be bypassed substituting $\widetilde{V}^a_\mu$ with $Z_V V^a_\mu$ in eq. (7.2) and the relation is now valid up to order a^2 lattice artifacts. This relation allows for a determination of Z_V through

$$Z_V = \lim_{\mu_{\rm q}\to 0} \frac{-2\mu_{\rm q}\epsilon^{3ab}\sum_{\mathbf{x}}\langle P^b(x)P^b(0)\rangle}{\sum_{\mathbf{x}}\langle \tilde{\partial}_\mu V^a_\mu(x) P^b(0)\rangle} \qquad a = 1, 2\,, \tag{7.7}$$

where $\tilde{\partial}_\mu$ is the symmetric lattice derivative.

In fig. 23 there is an example of Z_V as a function of the quark mass for a quenched simulation [66] determined using eq. (7.7). It turns out that Z_V is to a good approximation linear in $(a\mu_{\rm q})^2$.

In contrast, the axial Ward identity does not hold in the bare theory. Axial Ward identities therefore provide normalization conditions which determine finite renormalization constants such as $Z_{\rm A}$, or finite ratios of scale dependent renormalization constants, such as $Z_{\rm S}/Z_{\rm P}$ [35].

As Wtm and standard Wilson quarks are not related by a lattice symmetry, the counterterm structure for composite fields with the same physical interpretation depends upon the twist angle ω, and a particular choice of ω can lead to substantial simplifications. A typical example is the computation of the pseudoscalar decay constant from the axial coupling to the pion. We have argued in sec. 2 that for renormalized correlation functions, the relation between physical and twisted basis can be inferred from the corresponding classical relations if the renormalization

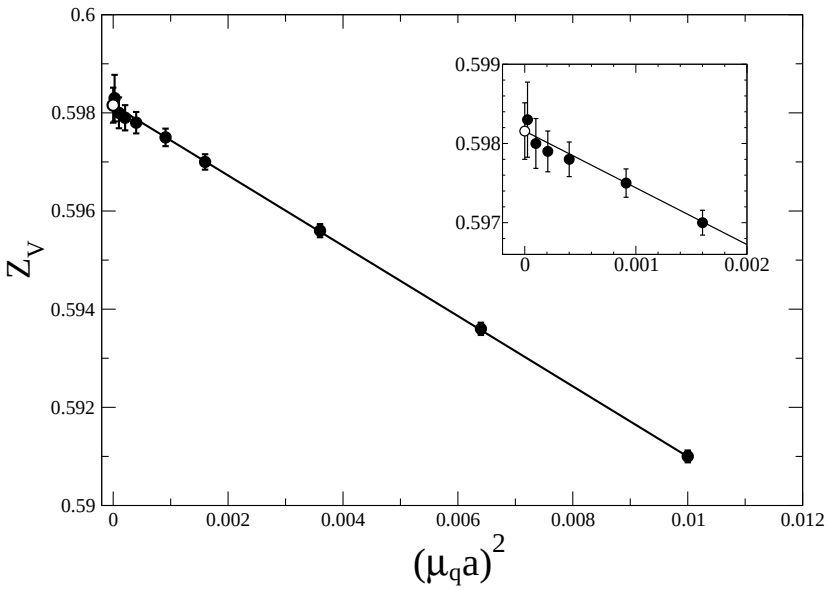


Fig. 23. An example of the extrapolation of Z_V to zero quark mass for a quenched simulation [66] at a lattice spacing of $a = 0.123$ fm. The data show a linear behaviour in $(a\mu_{\rm q})^2$.

scheme adopted is mass independent. With Wilson fermions usually the pseudoscalar decay constant is extracted from the correlation function

$$a^3 \sum_{\mathbf{x}} \langle (\mathcal{A}_{\rm R})^a_0(x) P^a_{\rm R}(0) \rangle. \tag{7.8}$$

This requires first the determination of the renormalized axial current and eventually all the relevant improvement coefficients. Performing the axial rotation (2.6) we obtain that in the continuum limit we should have (we set the isospin component $a = 1$)

$$\langle (\mathcal{A}_{\rm R})^1_0(x) P^1_{\rm R}(y) \rangle_{(M_{\rm R},0)} = \cos(\omega) \langle (A_{\rm R})^1_0(x) P^1_{\rm R}(y) \rangle_{(m_{\rm R},\mu_{\rm R})} + \sin(\omega) \langle V^2_0(x) P^1_{\rm R}(y) \rangle_{(m_{\rm R},\mu_{\rm R})}. \tag{7.9}$$

If we set $\omega = \pi/2$ the r.h.s of eq. (7.9) only contains the vector current which is protected against renormalization. Moreover using the exact PCVC relation on the lattice (7.2) it is easy to show [53, 85, 88] that

$$f_{\rm PS} = \frac{2\mu_{\rm q} |\langle \Omega | \hat{P}^a | {\rm PS} \rangle|}{M^2_{\rm PS}} \qquad a = 1, 2, \tag{7.10}$$

where $M_{\rm PS}$ is the charged pseudoscalar mass and $|{\rm PS}\rangle$ denotes the corresponding pseudoscalar state. As we see, the neat result is that Wtm at full twist allows the determination of an automatically O(a) improved pseudoscalar decay constant without the knowledge of any renormalization constant and any improvement coefficient.

In fig. 24, I summarize Wtm results coming from quenched [66,95] ($N_f = 0$) and unquenched [69] ($N_f = 2$) simulations, for the pseudoscalar decay constant over a range of pseudoscalar masses around $[300 - 700]$ MeV. We recall that for Wtm, to produce

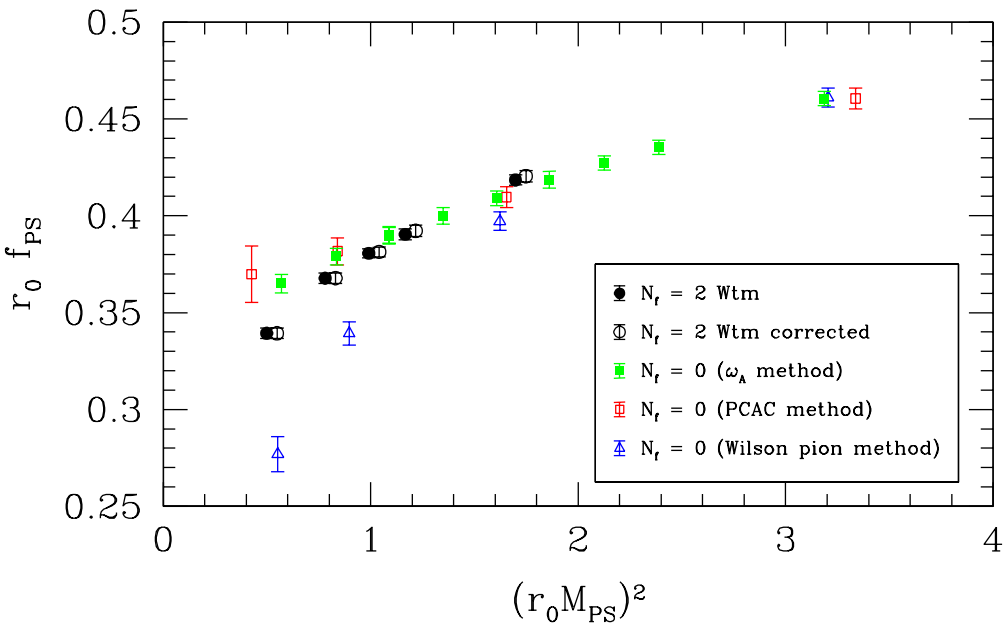


Fig. 24. Summary of the Wtm numerical results at $\omega = \pi/2$ for the pseudoscalar decay constant $f_{\rm PS}$ as a function of $M^2_{\rm PS}$. The bending phenomenon is visible with the "Wilson pion" definition of the critical mass for $N_f = 0$. The corrected data for $N_f = 2$ (slightly displayed for clarity) include the effect of the non vanishing $m_{\rm PCAC}$ (7.11). The perfect consistency of the data dispels all the doubts about the possible origins of the mass dependence for $f_{\rm PS}$.

such a plot, no renormalization constant are needed. Even if the lattice spacing for the quenched ($a = 0.093$ fm) and the unquenched ($a = 0.087$ fm) simulations are not exactly the same, it is interesting to notice the effect of the dynamical quarks in the mass dependence of the pseudoscalar decay constant. Moreover I also plot for the dynamical case the pseudoscalar decay constant corrected using eq. (4.83) and using the PCAC quark mass determined in the same set of simulations

$$f^{\rm corr}_{\rm PS} = f_{\rm PS} \frac{\sqrt{\mu_{\rm q}^2 + m^2_{\rm PCAC}}}{\mu_{\rm q}}. \tag{7.11}$$

In the statistical errors the two results are perfectly consistent showing that the mass dependence of $f_{\rm PS}$ for $N_f = 2$ is a genuine $\mu_{\rm q}$ quark mass dependence and and the curvature is not artificially induced by a non exactly zero PCAC mass. As a comparison I show also the $N_f = 0$ results obtained with the "Wilson pion" definition of the critical mass, where, on the contrary, the quark mass dependence

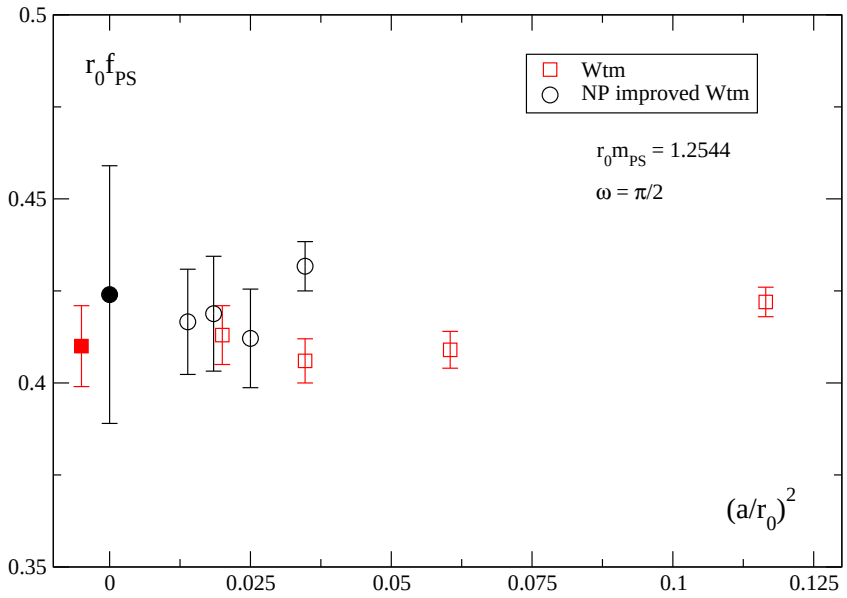


Fig. 25. Comparison of the continuum limit (filled symbols) at $r_0 M_{\rm PS} = 1.2544$ obtained in Wtm at full twist without [66] (red squares) and with [72] (black circles) improvement coefficients.

is largely given by the cutoff effects, as discussed in sect. 4.

In ref. [66, 72] the continuum limit of the quenched data is performed at $\omega = \pi/2$ producing consistent results. In fig. 25 we see an example of the two continuum limits for a pseudoscalar mass fixed at the kaon mass ($r_0 M_{\rm PS} = 1.2544$). While in ref. [66] no improvement coefficients were used, in ref. [72] the whole set of improvement coefficients were used ($c_{\rm SW}$, $c_{\rm A}$,...) in the computation of the decay constant from various lattice definitions. Some of the improvement coefficients are known only at one loop, but obviously at full twist they are actually irrelevant. The data shown in fig. 25 corresponds to a definition involving only $c_{\rm SW}$ and $\tilde{b}_{\rm V}$ (this is the coefficient multiplying the O(a) counterterm in eq. (D.15)). From the plot it is evident how automatic O(a) improvement makes the usage of the improvement coefficients not relevant for the cancellation of the O(a) discretization errors. In ref. [66] the continuum limit is performed over a wide range of quark masses as discussed in sect. 4.5 of this review (e.g. see fig. 7). In ref. [72] several definitions of the decay constant allow to perform a constrained continuum limit with a final result which has a relative error smaller than 2%.

The very precise unquenched data down to pseudoscalar masses around 300 MeV [69]

allow a discussion of whether χPT formulæ can reproduce the mass dependence for $am_{\rm PS}$ and $af_{\rm PS}$. One possible source of systematic uncertainty is the finite size effects, and this can be taken into account using χPT. In particular the lowest two quark masses turn out to be significantly affected. Preliminary results at a smaller lattice spacing [90,91] show small discretization errors, indicating that discretization errors are under control. Therefore one could try to use continuum χPT to describe consistently the dependence of the data both on the finite spatial size (L) and on the quark mass $\mu_{\rm q}$.

The fit to the raw data for $M_{\rm PS}$ and $f_{\rm PS}$ has been performed simultaneously with the appropriate ($N_f = 2$) χPT formulæ [132, 133]

$$M^2_{\rm PS}(L) = 2B_0\mu_{\rm q}\,\left[1+\frac{1}{2}\xi\tilde{g}_1(\lambda)\right]^2\,\left[1+\xi\log(2B_0\mu_{\rm q}/\Lambda_3^2)\right]\,, \tag{7.12}$$

$$f_{\rm PS}(L) = F\,\left[1-2\xi\tilde{g}_1(\lambda)\right]\,\left[1-2\xi\log(2B_0\mu_{\rm q}/\Lambda_4^2)\right]\,, \tag{7.13}$$

where

$$\xi = 2B_0\mu_{\rm q}/(4\pi F)^2\,, \qquad \lambda = \sqrt{2B_0\mu_{\rm q}L^2}\,. \tag{7.14}$$

The finite size correction function $\tilde{g}_1(\lambda)$ was first computed by Gasser and Leutwyler in ref. [132] and is also discussed in ref. [133]. In eqs. (7.12) and (7.13) NNLO χPT corrections are assumed to be negligible. The formulæ above depend on four unknown parameters, B_0, F, Λ_3 and Λ_4, which will be determined by the fit. For details about the data analysis I refer to the original paper [69].

For the lightest four values of $a\mu_{\rm q}$, an excellent fit to the data on $f_{\rm PS}$ and $M_{\rm PS}$ is found (see figures 26 and 27). The fitted values of the four parameters are

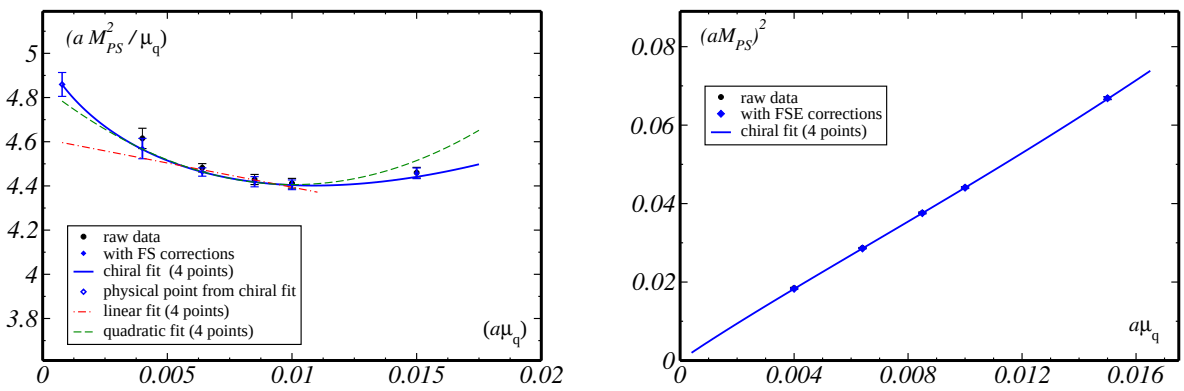
$$\begin{aligned} 2aB_0 &= -4.99(6)\,,\\ aF &= -0.0534(6)\,,\\ \log(a^2\Lambda_3^2) &= -1.93(10)\,,\\ \log(a^2\Lambda_4^2) &= -1.06(4)\,. \end{aligned} \tag{7.15}$$

The data are clearly sensitive to Λ_3 as visualized in figure 26(a).

The value of $a\mu_{\rm q}$, $a\mu_\pi$, at which the pion assumes its physical mass, is determined [69] requiring that the ratio $[\sqrt{[M^2_{\rm PS}(L=\infty)]}/f_{\rm PS}(L=\infty)]$ takes the value $(139.6/130.7) = 1.068$. From the knowledge of $a\mu_\pi$ one can evaluate
$\bar{l}_{3,4} \equiv \log(\Lambda^2_{3,4}/M^2_{\rm PS})|_{M_{\rm PS}=m_\pi}$

$$a\mu_\pi = 0.00078(2), \qquad \bar{l}_3 = 3.65(12), \qquad \bar{l}_4 = 4.52(06). \tag{7.16}$$

These results compare nicely with other determinations (for a review see ref. [134]). The inclusion of the results from $a\mu_{\rm q} = 0.0150$ in the fit gives an acceptable description of $M^2_{\rm PS}$ but misses the data for $f_{\rm PS}$, as shown in figures 26(b) and 27. Note,



(a) (b)

Fig. 26. In (a) I plot $(aM_{\rm PS})^2/(a\mu_{\rm q})$ as a function of $a\mu_{\rm q}$. In addition the χPT fit with eq. (7.12) to the data from the lowest four values of $\mu_{\rm q}$ is compared with linear and quadratic fits. In (b) I plot $(aM_{\rm PS})^2$ as a function of $a\mu_{\rm q}$ with the corresponding chiral fit. In both figures (a) and (b) the raw and the finite size corrected ($L \to \infty$) data are plotted.

however, that in Eqs. (7.12, 7.13), and thus in the fit results (7.15, 7.16), a number of systematic errors, as discussed below, are not included.

The values presented here should hence be taken as a first estimate, the validity of which has to be checked in the future. Nevertheless, the statistical accuracy achieved implies that there is a very good prospect of obtaining accurate and reliable values for the low-energy constants from Wtm fermion simulations.

Based on the physical value of f_π, one gets

$$a = 0.087(1)\ \text{fm}\,. \tag{7.17}$$

Using the value of r_0/a reported in ref. [69], this lattice calibration method yields $r_0 = 0.454(7)$ fm.

We now discuss the possible sources of systematic error. This analysis is based on lattice determinations of properties of pseudoscalar mesons with masses in the range 300 to 500 MeV on lattices with a spatial size slightly above 2 fm. Systematic errors can arise from several sources:

(i) Finite lattice spacing effects. Preliminary results at a smaller value of the lattice spacing that were presented in refs. [90,91] suggest that $\mathcal{O}(a)$ improvement is nicely at work and that residual $\mathcal{O}(a^2)$ effects are small.

(ii) Finite size effects (FSE). Even if the results presented here are obtained from a

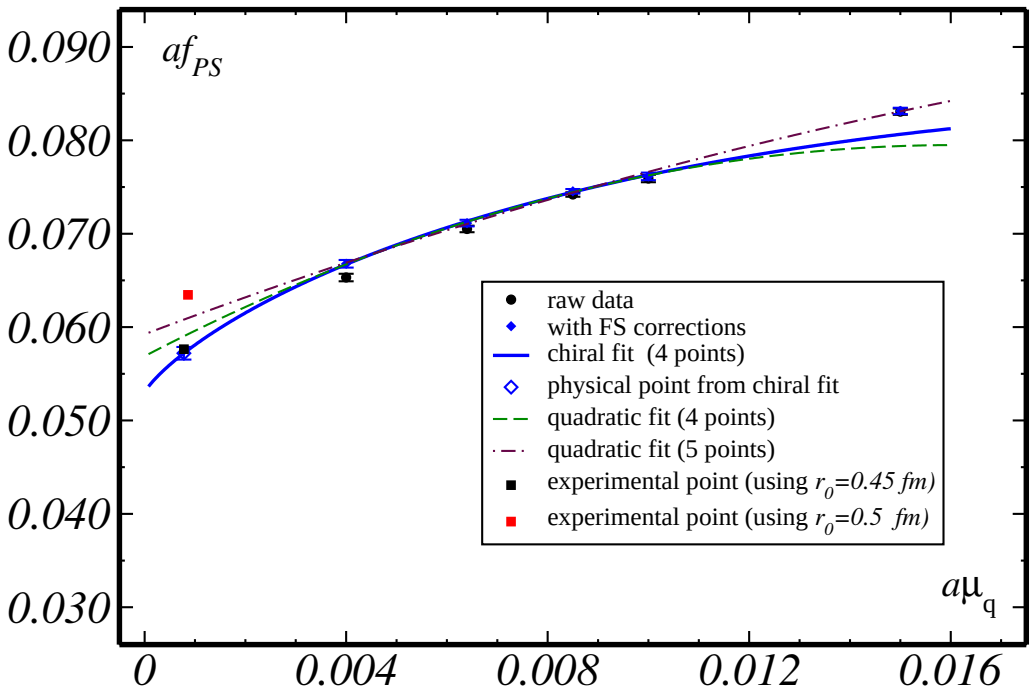


Fig. 27. Plot of $af_{\rm PS}$ (before and after finite size corrections) as a function of $a\mu_{\rm q}$ together with a fit to χPT formula (7.13). This fit is compared with a quadratic fit including all the data points and excluding the heaviest mass. A comparison with the impact of different physical values for r_0 is also shown.

box of physical size $L \gtrsim 2$ fm, to check that next to leading order (continuum) χPT adequately describes the FSE, a run on a larger lattice is required.

(iii) Mass difference of charged and neutral pseudoscalar meson. In the appropriate WχPT power counting for our values of the lattice spacing and quark masses, i.e. $\mu_{\rm R} \sim p^2 \sim a$ (4.67), the pion mass splitting is a NLO effect $(M_{\pi^\pm})^2 - (M_{\pi^0})^2 = \mathcal{O}(a^2\Lambda^4_{\rm QCD})$, from which it follows that to the order we have been working the effects of the pion mass splitting do not affect, in particular, the finite size correction factors for $M_{\rm PS}$ and $f_{\rm PS}$. In spite of these formal remarks, it is possible, however, that the fact that the neutral pion is lighter than the charged one (by about 20% at $a\mu_{\rm q} = 0.0040$, see ref. [69]) makes inadequate the continuum χPT description of finite size effects adopted in the present analysis. This caveat represents a further motivation for simulations on larger lattices, which will eventually resolve the issue.

(iv) Extrapolation to physical quark masses. We are assuming that χPT at next

to leading order for the $N_f = 2$ case is appropriate to describe the quark mass dependence of M_{PS}^2 and f_{PS} up to ~ 450–500 MeV. The lattice data are consistent with this, but it would be useful to include higher order terms in the χPT fits as well as more values of $a\mu_q$ to check this assumption. The effect of heavier quarks in the sea should also be explored, and preparatory studies with $N_f = 2 + 1 + 1$ [41] dynamical quarks show that the inclusion of heavier quarks in dynamical simulations is accessible using current algorithms and machines.

7.2 B_K

Indirect CP violation in $K \to \pi\pi$ decays is measured by the parameter ε_K, defined in terms of kaon decay amplitudes as

$$\varepsilon_K = \frac{T(K_L \to (\pi\pi)_{I=0})}{T(K_S \to (\pi\pi)_{I=0})}\,, \tag{7.18}$$

where I is the total isospin of the two-pion state. The long distance non-perturbative QCD contribution to $|\varepsilon_K|$ is provided by the following matrix element

$$B_K = \frac{\langle \bar{K}^0 | O_R^{\Delta S=2} | K^0 \rangle}{\frac{8}{3} f_K^2 M_K^2}\,, \tag{7.19}$$

where $O_R^{\Delta S=2}$ is the effective four-quark interaction renormalized operator, with bare operator

$$O^{\Delta S=2} = (\bar{s}\gamma_\mu^L d)(\bar{s}\gamma_\mu^L d)\,, \tag{7.20}$$

where $\gamma_\mu^L = \gamma_\mu(\mathbb{1} - \gamma_5)$. B_K largely dominates the uncertainty on the standard model (SM) value for $|\varepsilon_K|$ and improving the accuracy of B_K is essential in order to derive stringent bounds on the amount of non-SM CP violation in kaon decay.

One of the important sources of uncertainty in lattice QCD computations of B_K with Wilson fermions arises from operator renormalization. The operator $O^{\Delta S=2}$ is usually split into parity-even and parity-odd parts as

$$O^{\Delta S=2} = O_{\mathrm{VV+AA}} - O_{\mathrm{VA+AV}}, \tag{7.21}$$

where with obvious notation we have

$$O_{\mathrm{VV+AA}} = (\bar{s}\gamma_\mu d)(\bar{s}\gamma_\mu d) + (\bar{s}\gamma_\mu\gamma_5 d)(\bar{s}\gamma_\mu\gamma_5 d)\,, \tag{7.22}$$

$$O_{\mathrm{VA+AV}} = (\bar{s}\gamma_\mu d)(\bar{s}\gamma_\mu\gamma_5 d) + (\bar{s}\gamma_\mu\gamma_5 d)(\bar{s}\gamma_\mu d)\,. \tag{7.23}$$

Since parity is a QCD symmetry, the only contribution to the K^0–$\bar{K}^0$ matrix element comes from $O_{\mathrm{VV+AA}}$. In regularizations which respect chiral symmetry, the latter operator is multiplicatively renormalizable. If chiral symmetry is not preserved, $O_{\mathrm{VV+AA}}$ mixes with four other dimension-6 operators [135–137] with positive parity:

$$(O_{\rm R})_{\rm VV+AA}(\mu) = Z_{\rm VV+AA}(g_0, a\mu)\Big[O_{\rm VV+AA}(g_0) + \sum_{i=1}^{4} \Delta_i(g_0) O_i(g_0)\Big]. \tag{7.24}$$

The operators $O_i(g_0)$ belong to different chiral representations than $O_{\rm VV+AA}$. The mixing coefficients $\Delta_i(g_0)$ are finite functions of the bare coupling, while the renormalization constant $Z_{\rm VV+AA}$ diverges logarithmically in $a\mu$, where μ is the renormalization scale.

There have been several proposals to eliminate this operator mixing with Wilson fermions, all based on the observation [137, 138] that, even in the absence of chiral symmetry, the operator $O_{\rm VA+AV}$ is protected from finite operator mixing by discrete symmetries, and thus it renormalizes multiplicatively

$$(O_{\rm R})_{\rm VA+AV}(\mu) = Z_{\rm VA+AV}(g_0, a\mu) O_{\rm VA+AV}(g_0)\,. \tag{7.25}$$

In order to show this, it is convenient to work with massless Wilson fermions, also having in mind a mass independent renormalization scheme.

First of all we note that $O^{\Delta S=2}$ cannot mix with operators of lower dimensionality, because such operators do not have the four-flavour content of the original one. Thus $O^{\Delta S=2}$ can mix with any other dimension-six operator, provided it has the same quantum numbers, i.e. with any operator which has the symmetries of $O^{\Delta S=2}$ and of the lattice action. The generic QCD Wilson lattice action with 4 massless quarks is symmetric under parity $\mathcal{P}$ defined in eq. (2.34), and charge conjugation $\mathcal{C}$ (see app B for the definition). We define the generic four fermion operators

$$O_{\Gamma^{(1)}\Gamma^{(2)}} = (\overline{\chi}_1 \Gamma^{(1)} \chi_2)(\overline{\chi}_3 \Gamma^{(2)} \chi_4) \tag{7.26}$$

for all $\Gamma^{(1)}$ and $\Gamma^{(2)}$ combinations of interest. Moreover, there are other useful (flavour) symmetries of the action, namely the switching symmetries $\mathcal{S}'$ and $\mathcal{S}''$ defined by [138]

$$\mathcal{S}' : \begin{cases} \chi_1 \leftrightarrow \chi_2, \\ \chi_3 \leftrightarrow \chi_4 \end{cases} \tag{7.27}$$

$$\mathcal{S}'' : \begin{cases} \chi_1 \leftrightarrow \chi_4, \\ \chi_2 \leftrightarrow \chi_3. \end{cases} \tag{7.28}$$

In Table 1 I classify the operators $O_{\Gamma^{(1)}\Gamma^{(2)}}$, for all $\Gamma^{(1)}$ and $\Gamma^{(2)}$ with negative parity, according to the discrete symmetries $\mathcal{C}$, $\mathcal{S}'$ and $\mathcal{S}''$, with notation

$$O_{\Gamma^{(1)}\Gamma^{(2)} \pm \Gamma^{(2)}\Gamma^{(1)}} = O_{\Gamma^{(1)}\Gamma^{(2)}} \pm O_{\Gamma^{(2)}\Gamma^{(1)}}\,. \tag{7.29}$$

Parity violating operators, for which $\mathcal{C}\mathcal{S}''$ is not a symmetry, have been symmetrized or antisymmetrized in order to obtain eigenstates of $\mathcal{C}\mathcal{S}''$.

$O_{\Gamma^{(1)}\Gamma^{(2)}}$	$\mathcal{P}$	$\mathcal{CS}'$	$\mathcal{CS}''$	$\mathcal{CPS}'$	$\mathcal{CPS}''$
O_{VA+AV}	-1	-1	-1	$+1$	$+1$
O_{VA-AV}	-1	-1	$+1$	$+1$	-1
O_{SP-PS}	-1	$+1$	-1	-1	$+1$
O_{SP+PS}	-1	$+1$	$+1$	-1	-1
$O_{T\tilde{T}}$	-1	$+1$	$+1$	-1	-1

Table 1
Classification of parity violating four-fermion operators $O_{\Gamma^{(1)}\Gamma^{(2)}}$ according to useful products of discrete symmetries $\mathcal{P}$, $\mathcal{C}$, $\mathcal{S}'$ and $\mathcal{S}''$. Note that $O_{\tilde{T}\tilde{T}} = O_{TT}$ and $O_{T\tilde{T}} = O_{\tilde{T}T}$.

The parity violating four- fermion operators listed in table 1 do not all have identical $\mathcal{CPS}'$ and $\mathcal{CPS}''$ values. It is straightforward to see that the operator O_{VA+AV} cannot mix with the other parity violating operators [20] .

We are going now to discuss two possible approaches [98, 139] which use Wtm to extract the renormalized $\langle \bar{K}^0 | O_{\rm VV+AA} | K^0 \rangle$ by relating it to the matrix element of a parity violating operator. As the Wtm action differs from the standard Wilson fermion action by the mass term, the renormalization properties of composite operators in mass independent renormalization schemes are not modified. In particular, $O_{\rm VA+AV}$ remains multiplicatively renormalizable, with the same renormalization constant and running as with Wilson fermions. Thus finite subtractions are avoided in the Wtm determination of B_K. In order to disentangle the two approaches we will call the proposal made in [70, 139] the "mixed twist" method while the proposal in [98] the "mixed action" method. Hopefully the reasons for these names will become clear in the following.

7.2.1 "Mixed twist" method

The first variant of the "mixed twist" method consists in choosing the following fermionic action

$$S_{\rm F}^{(\pi/2)} = a^4 \sum_x \left[\overline{\chi}(x)(D_{\rm w,sw} + m_l + i\gamma_5 \tau^3 \mu_l)\chi(x) \; + \; \bar{s}(x)(D_{\rm w,sw} + m_s)s(x) \right]. \quad (7.30)$$

where $D_{\rm w,sw}$ is the clover improved Wilson operator (4.18,4.19) and χ collects the light doublet

$$\chi = \begin{pmatrix} u \\ d \end{pmatrix}.$$

[20] It could still mix with the Fierz transformed in Dirac space operator O^F_{VA+AV}. It turns out that $O^F_{VA+AV} = O_{VA+AV}$ (see ref. [137] for details).

The label $\pi/2$ refers to the choice of the twist angle that can be obtained setting $m_{\mathrm{R},l} = 0$. We see that while the twist angle of the first doublet is $\pi/2$, the twist angle of the strange quark is zero, hence the name "mixed twist".

The second variant is based on the action

$$S_{\mathrm{F}}^{(\pi/4)} = a^4 \sum_x \left[\bar{u}(x)(D_{\mathrm{w,sw}} + m_u)u(x) \; + \; \overline{\chi}(x)(D_{\mathrm{w,sw}} + m_l + i\gamma_5\tau^3\mu_l)\chi(x)\right]. \quad (7.31)$$

where now χ collects a doublet made of a *down* and a *strange* quark

$$\chi = \begin{pmatrix} s \\ d \end{pmatrix}.$$

To set now the twist angle to $\pi/4$ requires $\mu_{\mathrm{R},l} = m_{\mathrm{R},l}$. The variant with action (7.31) assumes *a priori* that the s and d quarks have degenerate physical masses. This is necessary if one would like to extend this variant to unquenched simulations: a non degenerate diagonal twisted doublet would lead to a complex determinant [39]. As long as this action is used in quenched QCD this restriction is not needed but all the computations carried out with it are performed with degenerate s and d quarks. The action in eq. (7.30), on the other hand, is perfectly well suited for an unquenched computation.

It is important to stress that in both the variants not all the quark flavours are fully twisted, i.e. automatic O(a) improvement [11] does not apply. To have full O(a) improvement of the matrix element it would be necessary to subtract a number of dimension-seven counterterms from the four-fermion operator. Such a procedure is highly impractical, and has not been pursued. Hence leading cutoff effects in B_K with the "mixed twist" methods are expected to be linear in a.

We have already discussed in sect. 2, that to relate renormalized correlation functions computed with tmQCD to QCD, it is enough to perform the needed change of variables (axial rotations). This explains the choice of the twist angles for the two variants. In fact performing the rotation in eq. (2.6) for the two actions, we obtain in both cases

$$\langle K^0| \, (O_R)_{\mathrm{VV+AA}} \, |\bar{K}^0\rangle_{\mathrm{QCD}} = -i\langle K^0| \, (O_R)_{\mathrm{VA+AV}} \, |\bar{K}^0\rangle_{\mathrm{tmQCD}}\,, \quad (7.32)$$

which holds in the continuum limit for the two versions of Wtm under consideration. From this identity, B_K can be extracted from a K^0–$\bar{K}^0$ matrix element of the multiplicatively renormalizable operator $O_{\mathrm{VA+AV}}$.

Both these variants has been used to compute B_K with quenched fermions.

In particular the non-perturbative renormalization has been performed in the SF

scheme [140], and the matrix element has been computed using both the variants in quenched simulations [70, 72]. The twist angle has been tuned to $\omega = \pi/2$ setting $m_{\mathrm{R},l} = 0$ in the clover improved theory. This corresponds to the full twist tuning discussed in sect. 4.3.1. To tune the twist angle to $\pi/4$, the untwisted quark mass has been tuned such that $\mu_{\mathrm{R},l} = m_{\mathrm{R},l}$, which via eqs. (4.22,4.23) and eqs. (4.25,4.26) translates into

$$am_{q,l} = \frac{Z_\mu}{Z_m} a\mu_l \Big\{ 1 + \Big[\frac{Z_\mu}{Z_m}(b_\mu - b_m) - \frac{Z_m}{Z_\mu}\tilde{b}_m \Big] a\mu_l \Big\} \tag{7.33}$$

For a given choice of $a\mu_l$, $\kappa = (2am_l + 8)^{-1}$ is tuned so that $am_{q,l}$ satisfies one of the two above relations. This requires the knowledge of all the renormalization constants and improvement coefficients. The final result for the renormalization group invariant matrix element $\hat{B}_K$ being

$$\hat{B}_K = 0.735(71). \tag{7.34}$$

The only systematic uncertainty that affects this computation is the usage of quenched fermions.

In fig. 28 we summarize results for $\hat{B}_K$ obtained by several collaborations using different lattice actions. In particular we observe that Wtm allows a very precise determinations of $\hat{B}_K$ which is competitive with the determination obtained with other discretizations. The main drawback of the "mixed twist" approach is the fact that the leading cutoff effects in B_K are expected to be linear in a.

7.2.2 "Mixed action" method

The second method we are going to discuss has all the quark flavours at full twist, thus retaining automatic $\mathrm{O}(a)$ improvement, but it makes use of different lattice actions for valence and sea quarks. In particular the valence actions are chosen in order to remove the unwanted mixings for $O_{\mathrm{VA+AV}}$. To obtain this goal the number of valence quarks has to be extended, i.e. some of the valence quarks involved in the correlation function under investigation have to be doubled with a slightly different lattice action. The resulting lattice theory is not unitary thus the approach to the continuum limit will be affected by $\mathrm{O}(a^2)$ effects coming from unitarity violations. With the "mixed action" a detailed understanding of these particular discretization errors have to be achieved in order to correctly perform the continuum limit. This does not pose any problem of principle because once the renormalized quark masses, or equivalently the corresponding pseudoscalar meson masses, are matched in the continuum limit, one obtains the desired and correct renormalized matrix element. [21]

[21] This statement could be put at a more formal level using a Ginsparg-Wilson regularization.

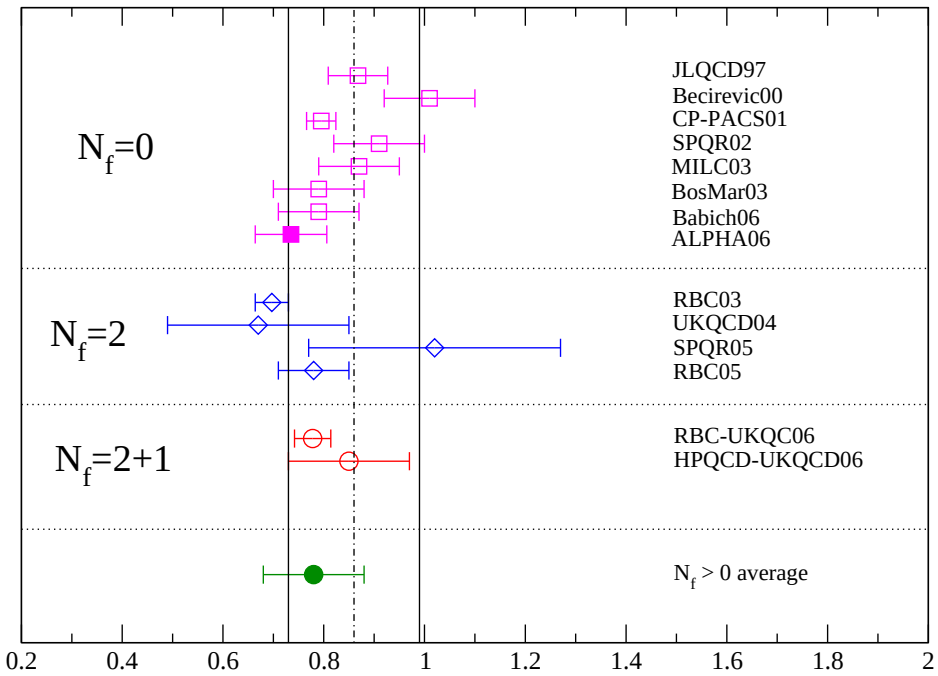


Fig. 28. Summary plot of the results for $\hat{B}_K$ obtained by several collaborations using different lattice actions. From the top to the bottom the refs. are [72,141–153]. The $N_f = 0$ Wtm result [72] is shown with a filled square.

For the light (l) and the heavy (h) sea doublet quarks the actions are [22]

$$S^{(l)}_{\rm Wtm} = a^4 \sum_x \overline{\chi}_l(x) \Big[D_{\rm W} + m_0 + i\mu_l \gamma_5 \tau^3 \Big] \chi_l(x), \tag{7.35}$$

$$S^{(h)}_{\rm Wtm} = a^4 \sum_x \overline{\chi}_h(x) \Big[D_{\rm W} + m_0 + i\mu_h \gamma_5 \tau^3 + \epsilon_h \tau^1 \Big] \chi_h(x), \tag{7.36}$$

For the particular case of B_K we introduce the following valence quarks: d, s and s'. The d and the s valence quarks have the Osterwalder-Seiler (OS) action

$$S^{(f)}_{\rm OS} = a^4 \sum_x \overline{\chi}_f(x) \Big[D_{\rm W} + m_0 + i\mu^v_f \gamma_5 \Big] \chi_f(x), \tag{7.37}$$

[22] In principle it is possible to choose also a non-degenerate quark action for the light sector.

with $f = d, s$ while the s' quark has the same OS action

$$S_{\rm OS}^{(s')} = a^4 \sum_x \bar{s}'(x) \Big[D_{\rm W} + m_0 - i\mu_{s'}^v \gamma_5 \Big] s'(x), \tag{7.38}$$

but with an opposite sign for the mass term. While this certainly does not change the sign of the physical quark mass, it changes the leading discretization errors of the actions, in such a way that to extract B_K it is possible to use a specific correlation function that renormalizes multiplicatively and it is automatically O(a) improved.

The OS action differs from Wtm by the fact that it does not violate isospin. This action is not used for dynamical fermions since, as we have discussed in sect. 2, it could generate an $F\widetilde{F}$ in the renormalization process through vacuum polarization diagrams. Because of the peculiar flavour structure, this does not happen for Wtm, but anyhow the OS action can be still used for valence quarks. To correctly define the theory we would need to introduce for each valence quark, the corresponding ghost action which cancels exactly the contribution to the determinant [154]. We will assume that this it has been done. All the considerations which follow will not involve correlation functions of ghost fields, thus the standard Symanzik expansion will apply [155], and all the symmetries we are going to use will be naturally extended to the ghost fields.

We reiterate that the valence and sea quark masses have to be correctly matched to obtain the correct continuum limit. We also recall that to obtain automatic O(a) improvement the untwisted quark mass has to be tuned to the critical value, and so the physical quark mass is totally given by the twisted quark mass. This is obtained with the following matching prescription

$$\begin{aligned} (\mu_d)_{\rm R} &= (\mu_d^v)_{\rm R}, \\ (\mu_s)_{\rm R} &= (\mu_s^v)_{\rm R} = (\mu_{s'}^v)_{\rm R}. \end{aligned} \tag{7.39}$$

With the choice of the valence quark actions specified in eqs. (7.37,7.38), it is easy to show, performing the usual axial rotations, that the original matrix element

$$\langle \overline{K}^0 | O_{\rm R}^{\Delta S=2} | K^0 \rangle_{\rm QCD} = \frac{8}{3} M_K^2 f_K^2 B_K \tag{7.40}$$

is equivalent to the matrix element

$$\langle \overline{K}'^0 | 2(\mathcal{O}_{\rm R})_{VA+AV} | K^0 \rangle = \frac{8}{3} M_K M_{K'} f_K f_{K'} B_K \tag{7.41}$$

where this second matrix element on the lattice is computed with the model specified before. In particular the bare operator reads

$$\mathcal{O}_{VA+AV} = i \left[(\bar{s}\gamma_\mu d)(\bar{s}'\gamma_\mu\gamma_5 d) + (\bar{s}\gamma_\mu\gamma_5 d)(\bar{s}'\gamma_\mu d) \right] \tag{7.42}$$

and the interpolating fields for the kaons are

$$K^0(x) = i\bar{d}(x)s(x), \qquad \overline{K}'^0(x) = \bar{s}'(x)\gamma_5 d(x). \tag{7.43}$$

The matrix element (7.42) can then be extracted by the asymptotic behaviour of the correlation function

$$C_{K'OK}(x_0, y_0) = 2a^6 \sum_{\mathbf{x},\mathbf{y}} \langle (\bar{d}\gamma_5 s')(x) \mathcal{O}_{VA+AV}(0) (\bar{d}s)(y) \rangle, \tag{7.44}$$

with $y_0 < 0$ and $x_0 > 0$. The values of M_K,$M_{K'}$,f_K and $f_{K'}$, can be extracted in a standard fashion from the 2-point correlation functions involving the interpolating fields in (7.43). We repeat here briefly the reason why $\mathcal{O}_{VA+AV}$ is multiplicatively renormalized. Mixing with lower dimensional operators is excluded by flavour symmetry of the massless lattice actions, in particular $\mathcal{O}_{VA+AV}$ can mix only with operators such that $\Delta s = \Delta s' = -\Delta d/2 = 1$. Parity symmetry of the action in the chiral limit forbids mixing with operators of the opposite parity. Possible dimension 6 operators of negative parity that could mix with $\mathcal{O}_{VA+AV}$ are

$$O_{VA-AV} = (\bar{s}\gamma_\mu d)(\bar{s}'\gamma_\mu\gamma_5 d) - (\bar{s}\gamma_\mu\gamma_5 d)(\bar{s}'\gamma_\mu d) \tag{7.45}$$

$$O_{SP\pm PS} = (\bar{s}d)(\bar{s}'\gamma_5 d) \pm (\bar{s}\gamma_5 d)(\bar{s}'d) \tag{7.46}$$

$$O_{T\tilde{T}} = \epsilon_{\mu\nu\lambda\rho}(\bar{s}\sigma_{\mu\nu}d)(\bar{s}'\sigma_{\lambda\rho}d) \tag{7.47}$$

To rule out these operators is enough to use $\mathcal{CPS}'$ and $\mathcal{CPS}''$ symmetries defined in eqs. (7.27,7.28), as we have done previously.

The main advantages of this approach is that all the quarks are at full twist so to prove automatic O(a) improvement it is enough to generalize the form of the *twisted parity* used in sect. 4

$$\mathcal{P}_{\frac{\pi}{2}}: \begin{cases} U(x_0,\mathbf{x};0) \to U(x_0,-\mathbf{x};0), \quad U(x_0,\mathbf{x};k) \to U^{-1}(x_0,-\mathbf{x}-a\hat{k};k), \quad k=1,\,2,\,3 \\ \chi_{l,h}(x_0,\mathbf{x}) \to \gamma_0(i\gamma_5\tau^3)\chi_{l,h}(x_0,-\mathbf{x}) \\ \overline{\chi}_{l,h}(x_0,\mathbf{x}) \to \overline{\chi}_{l,h}(x_0,-\mathbf{x})(i\gamma_5\tau^3)\gamma_0 \\ q_f(x_0,\mathbf{x}) \to \gamma_0(i\gamma_5)q_f(x_0,-\mathbf{x}) \\ \bar{q}_f(x_0,\mathbf{x}) \to \bar{q}_f(x_0,-\mathbf{x})(i\gamma_5)\gamma_0, \end{cases} \tag{7.48}$$

where q_f generically indicates all the valence fields. Moreover non-degenerate quarks can be introduced retaining the nice property of a real and positive definite determinant [38]. This approach requires care in the matching procedure between valence and sea quarks.

An obvious alternative to avoid renormalization problems consists in using regularizations with exact chiral symmetry. However, the computational costs involved

make it difficult to perform continuum limit extrapolations and study finite volume effects. A first attempt using Wtm sea and overlap valence quarks has been presented at the last lattice conference [156].

We reiterate that one drawback of the mixed action approach is that the resulting theory is not unitary at non-zero lattice spacing. This introduces peculiar $O(a^2)$ cutoff effects, that nevertheless can be described by mixed action chiral perturbation theory [157, 158]. This cutoff effects have been investigated thoroughly in refs. [159, 160], and formulæ, valid up to $O(a^2)$, have been given for correlators computed with valence overlap fermions on a set of different sea quark actions.

The preliminary results of ref. [156] indicate that the whole procedure is limited by the statistical accuracy achievable on a large volume with overlap fermions, in order to correctly perform the matching procedure. A possible way to solve this problem is to match the current quark masses in a finite volume.

8 Algorithms for dynamical fermions

At present the only practical way to simulate numerically a 4–D euclidean quantum field theory with fermions is to perform the Grassmann integral on the fermion fields analytically and then to apply Monte Carlo methods in the resulting effective bosonic theory.

After integrating out the fermion fields $\chi, \overline{\chi}$ the partition function (2.22) of Wtm for $N_f = 2$ degenerate flavors is given by

$$\mathcal{Z} \propto \int \mathcal{D}U \det(Q^\dagger Q) e^{-S_{\rm G}[U]} = \int \mathcal{D}U e^{-S_{\rm eff}[U]} \ , \tag{8.1}$$

with

$$S_{\rm eff}[U] = S_{\rm G}[U] - {\rm Tr} \log Q^\dagger Q \ . \tag{8.2}$$

The reality of the effective action is only guaranteed by the positivity of the quark determinant.

8.1 Hybrid Monte Carlo

The determinant $\det(Q^\dagger Q)$ can be expressed in terms of the so called pseudofermion complex fields ϕ

$$\det(Q^\dagger Q) \propto \int \mathcal{D}\phi^\dagger \mathcal{D}\phi \exp\Big(-S_{\rm PF}[U, \phi^\dagger, \phi]\Big) \, , \tag{8.3}$$

where $S_{\rm PF}[U, \phi^\dagger, \phi] = (Q^{-1}\phi, Q^{-1}\phi)$ is the pseudofermion action with standard scalar product (u, v). The pseudofermion fields ϕ are formally identical to the fermion fields χ, but follow the statistics of bosonic fields.

A way to obtain a "good" global update with the non-local effective bosonic action $S_{\rm PF}$ is to simulate a *microcanonical ensemble* with a suitably defined Hamiltonian. The Hamilton equations have to be integrated with a suitable integration scheme, and it is then possible to correct for the the finite step errors with a final stochastic accept-reject step. This is schematically what is called the Hybrid Monte Carlo (HMC) algorithm [161]. To be more specific, the ϕ version of the HMC algorithm is based on the Hamiltonian

$$H(\Pi, U, \phi, \phi^\dagger) = \frac{1}{2} \sum_{x,\mu} {\rm Tr}[\Pi(x,\mu)^2] + S_{\rm G}[U] + S_{\rm PF}[U, \phi, \phi^\dagger] \, , \tag{8.4}$$

where we introduced traceless hermitian momenta $\Pi(x, \mu)$. The HMC algorithm is then composed by the following steps

- Global heat-bath for momenta and pseudofermion fields:
  the initial momenta are randomly chosen according to a Gaussian distribution $\exp(-\Pi^2/2)$, and the random fields R are produced from a distribution like $\exp(-R^\dagger R)$with the initial pseudofermions computed as $\phi = Q \cdot R$.
- Molecular dynamics evolution:
  propose a gauge configuration U' and a momentum Π' integrating the Hamilton equations of motion for the gauge field U and the momentum Π at fixed pseudofermion field ϕ.
- Metropolis accept/reject step:
  The proposals U' and Π' are accepted with probability $\min\{1, \exp(-\Delta H)\}$, where $\Delta H = H(\Pi', U', \phi, \phi^\dagger) - H(\Pi, U, \phi, \phi^\dagger)$. This step is needed because of the numerical inexact integration of the equations of motion.

It possible to prove that the HMC algorithm satisfies the *detailed balance* condition [161] and hence the configurations generated with this algorithm correctly represent the intended ensemble. Since the Hamiltonian is conserved up to finite step errors, the integration can be set up such that the gauge configurations are globally updated keeping the acceptance rate high.

8.2 Molecular dynamics evolution

In the molecular dynamics part of the HMC algorithm the gauge fields U and the momenta Π need to be evolved in a fictitious computer time τ. Differentiation on a compact Lie group is defined, given a generic function G, by

$$G[U\mathrm{e}^{i\omega_a T^a}] = G[U] + \omega_a \delta^a_\omega G[U] + O(\omega^2) \ , \tag{8.5}$$

where U is group element, ω is an infinitesimal vector with dimension equal to that of the adjoint representation and T^a are the group generators. Since the variation $\delta^a_\omega G$ takes values in the Lie algebra it is natural to let the momenta $\Pi(x,\mu)$ be an element of the Lie algebra. With respect to τ, Hamilton's equations of motion read

$$\frac{d}{d\tau}U(x,\mu) = \Pi(x,\mu)U(x,\mu) \ , \qquad \frac{d}{d\tau}\Pi(x,\mu) = -F(x,\mu) \ , \tag{8.6}$$

where the force $F(x,\mu)$ is obtained by differentiation with respect to the gauge links

$$(\omega, F) = \delta_\omega S \ , \qquad \delta_\omega U(x,\mu) = \omega(x,\mu)U(x,\mu) \tag{8.7}$$

and $S = S_{\mathrm{G}} + S_{\mathrm{PF}}$. Since analytical integration of the former equations of motion is normally not possible, these equations must in general be integrated with a discretized integration scheme that is area preserving and reversible. The discrete update with integration step size $\Delta\tau$ of the gauge field and the momenta can be

defined as

$$\begin{aligned} T_{\mathrm{U}}(\Delta\tau): \quad U \quad &\to \quad U' = E\left(i\Delta\tau\Pi(x,\mu)\right) U\,, \\ T_{\mathrm{S}}(\Delta\tau): \quad \Pi \quad &\to \quad \Pi' = \Pi - i\Delta\tau F\,, \end{aligned} \tag{8.8}$$

where $E(\cdot)$ stands for the $SU(3)$ exponential function. To integrate the equation of motion (8.8) it is possible to use many different integrators. One of the simplest is the so called leap-frog integrator. Given eq. (8.8) one basic time evolution step of the leap-frog reads

$$T = T_{\mathrm{S}}(\Delta\tau/2)\; T_{\mathrm{U}}(\Delta\tau)\; T_{\mathrm{S}}(\Delta\tau/2)\,, \tag{8.9}$$

and a whole trajectory of length τ is achieved by a number of molecular dynamics $N_{\mathrm{MD}} = \tau/\Delta\tau$ successive applications of the transformation T.

8.3 Preconditioning

For each step along a trajectory of length $\Delta\tau$ the force F has to be computed. The computation of the force F is the most expensive part in the HMC algorithm since the inversion of the Wilson-Dirac operator is needed. In order to improve the integration (i.e. to increase the step size $\Delta\tau$ or equivalently to reduce the number of steps N_{MD}) it would be better to have small forces along the trajectory. In general this is achieved by preconditioning the HMC algorithm. A good strategy would then be to split the forces in such a way that those which require more computer time to be computed are those with the smallest magnitude. When the chiral limit is approached, the quark forces tend to increase, which requires the step sizes to be adjusted accordingly [162], and the choice of the preconditioner can have an influence on this behaviour. A parameter that cannot be predicted in a dynamical simulation is the autocorrelation time of the quantity one is interested in. Extended simulations are needed in order to understand if the autocorrelation time is under control or not.

In general, preconditioning is always associated with a factorization of the quark determinant into the determinants of certain different operators. The number and the type of operators depend on the chosen preconditioner. A possible efficient preconditioning is obtained using a domain decomposition [163] (DD). The preconditioner we are going to discuss is the so called Hasenbusch acceleration or mass preconditioning [164]. From now on I will discuss only the case of the plain hermitian Wilson operator Q_W, because all the conclusions can be easily extended to the Wtm operator. It was realized in ref. [164] that using the identity

$$\det Q_W^2 = \det\left(Q_W^2 + \rho^2\right)\; \det\left(\frac{Q_W^2}{Q_W^2 + \rho^2}\right), \tag{8.10}$$

with an adjustable mass shift ρ, can speed up the HMC algorithm. Each of the two determinants on the r.h.s. of eq. (8.10) is treated by a separate pseudofermion field

ϕ_i and a corresponding pseudofermion action S_{PF_i}. The Hamiltonian can be written as

$$H = \frac{1}{2}\sum_{x,\mu} \mathrm{Tr}[\Pi(x,\mu)^2] + S_G + S_{\mathrm{PF}_1} + S_{\mathrm{PF}_2}\,. \tag{8.11}$$

where S_{PF_1} and S_{PF_2} are the pseudofermion actions respectively related to $\det\,(Q_W^2+\rho^2)$ and $\det\left(\frac{Q_W^2}{Q_W^2+\rho^2}\right)$.

In ref. [165,166] it was argued that the optimal choice for ρ is given by $\rho^2 = \sqrt{\lambda_{\mathrm{M}}\lambda_{\mathrm{m}}}$. Here λ_{M} (λ_{m}) is the maximal (minimal) eigenvalue of Q_W^2. The reason for that choice is obtained from minimizing the sum of the condition numbers $K = K_1 + K_2$ [23] for the operators appearing in S_{PF_1} and S_{PF_2}. With the optimal $\rho^2_{\mathrm{opt}} = \sqrt{\lambda_{\mathrm{M}}\lambda_{\mathrm{m}}}$ the two condition numbers K_1 and K_2 are equal to $\sqrt{\lambda_{\mathrm{M}}/\lambda_{\mathrm{m}}}$, both of them being smaller than the condition number of Q_W^2 which is $\lambda_{\mathrm{M}}/\lambda_{\mathrm{m}}$.

Since the force contribution in the molecular dynamics evolution is supposed to be proportional to some power of the condition number, the force contribution from the pseudofermion part in the action is reduced and therefore the step size $\Delta\tau$ can be increased, in practice by about a factor of 2 [164,165].

This preconditioning can be very easily adapted to the Wtm operator observing that $Q_W^2 + \rho^2 = Q^\dagger Q$ with ρ being the twisted mass and Q being γ_5 "times" the Wtm operators (2.66).

8.4 HMC with multiple time scale integration and mass preconditioning

In the paper by Lüscher [163] impressive acceleration factors were obtained with a DD preconditioned HMC compared with a plain HMC. One of the reasons for this impressive result is the observation that the resulting forces after the preconditioning have a magnitude which decreases as the computer time needed to invert the corresponding operator increases. It is then beneficial to integrate each single force with different time steps. This hierarchy of forces is obtained with a preconditioner that provides a strong infrared cutoff and separates low- and high-frequency modes of the system. In [167] the idea was explored of using as an infrared cutoff the mass in the Hasenbusch acceleration method, which could also give a similar hierarchy of forces that could then be combined with a suitable integrator. Therefore it might be advantageous to change the point of view: instead of tuning ρ à la refs. [164,165], i.e. minimizing the condition number of the operators appearing in the pseudofermion action, rather to exploit the possibility of arranging the forces by the help of mass

[23] The condition number is the ratio of the maximal over the minimal eigenvalue of a given operator.

preconditioning with the aim to reach a situation in which a multiple time scale integration scheme is favorable, i.e. tuning ρ to achieve a hierarchy of forces as with the DD-HMC.

The idea to combine a multiple time step integrator with a separation of infrared and ultraviolet modes was already proposed in ref. [168]. This idea was applied to mass preconditioning by using only two time scales in refs. [169,170] in the context of clover improved Wilson fermions. However, a comparison of results presented in the next section to the ones of refs. [169, 170] is not possible, because volume, lattice spacing and masses are different. The gain reported in [169] compared to the performance of the method described in [164, 165] was at most 20%.

In order to generalize the leap frog integration scheme (8.9) we assume, in the following, that we can bring the Hamiltonian to the form

$$H = \frac{1}{2}\sum_{x,\mu} \mathrm{Tr}[\Pi(x,\mu)^2] + \sum_{k=0}^{n} S_k[U]\,, \tag{8.12}$$

with $n \geq 1$. For instance with $n = 1$ S_0 might be identified with the gauge action and S_1 with the pseudofermion action of eq. (8.4).

Clearly, in order to keep the discretization errors small in an algorithm like leap frog, the time steps have to be small if the driving forces are large. Hence multiple time scale integration is a valuable tool, if the forces originating from the single parts in the Hamiltonian (8.12) differ significantly in their absolute values. Then the different parts in the Hamiltonian might be integrated on time scales inversely proportional to the corresponding forces.

The leap frog integration scheme can be generalized to multiple time scales as has been proposed in ref. [171] without loss of reversibility and the area preserving property. The scheme with only one time scale can be recursively extended by starting with the definition

$$T_0 = T_{\mathrm{S}_0}(\Delta\tau_0/2)\; T_{\mathrm{U}}(\Delta\tau_0)\; T_{\mathrm{S}_0}(\Delta\tau_0/2)\,, \tag{8.13}$$

with T_{U} defined as in eq. (8.8) and where $T_{\mathrm{S}_k}(\Delta\tau)$ is given by

$$T_{\mathrm{S}_k}(\Delta\tau_k) \quad : \quad P \quad \rightarrow \quad P - i\Delta\tau_k F_k\,. \tag{8.14}$$

As $\Delta\tau_0$ will be the smallest time scale, we can recursively define the basic update steps T_k, with time scales $\Delta\tau_k$ as

$$T_k = T_{\mathrm{S}_k}(\Delta\tau_k/2)\; [T_{k-1}]^{N_{k-1}}\; T_{\mathrm{S}_k}(\Delta\tau_k/2)\,, \tag{8.15}$$

with integers N_k and $0 < k \leq n$. One full trajectory τ is then composed by $[T_n]^{N_n}$. The different time scales $\Delta\tau_k$ in eq. (8.15) must be chosen such that the total number

of steps on the k-th time scale N_{MD_k} times $\Delta\tau_k$ is equal to the trajectory length τ for all $0 \leq k \leq n$: $N_{\mathrm{MD}_k}\Delta\tau_k = \tau$. This is achieved by setting

$$\Delta\tau_k = \frac{\tau}{N_n \cdot N_{n-1} \cdot \ldots \cdot N_k} = \frac{\tau}{N_{\mathrm{MD}_k}}\,, \qquad 0 \leq k \leq n\,, \tag{8.16}$$

where $N_{\mathrm{MD}_k} = N_n \cdot N_{n-1} \cdot \ldots \cdot N_k$.

In ref. [171] also a partially improved integration scheme with multiple time scales was introduced, which reduces the size of the discretization errors.

To summarize we decompose the pseudofermion action as

$$S = \sum_{k=0}^{n} S_k[U] \tag{8.17}$$

with

$$S_0 = S_G[U], \qquad S_1 = (Q_1^{-1}\phi_k, Q_1^{-1}\phi_k), \tag{8.18}$$

$$S_k = (Q_k^{-1}Q_{k-1}\phi_k, Q_k^{-1}Q_{k-1}\phi_k) \quad 1 \leq k \leq n \tag{8.19}$$

where

$$Q_k = Q_{\mathrm{W}} + i\rho_k \qquad \rho_k < \rho_{k-1} \tag{8.20}$$

and Q_n is the operator we are interested in: Q_{W} if we want to perform dynamical simulations with Wilson fermions or $Q_n = Q_{\mathrm{W}} + i\mu_{\mathrm{q}}$ if we want to perform simulation with Wtm ($\mu_{\mathrm{q}} < \rho_k \forall k$). The strategy is then to tune ρ_k and n in eq. (8.17) such that the more expensive the computation of a certain F_k is, the less it contributes to the total force. The different parts of the action can then be integrated on different time scales $\Delta\tau_k$ chosen according to their force magnitude F_k, guided by $\Delta\tau_k F_k = \text{const}$ for all k.

8.5 Results

In ref. [167,172] it was shown that this idea proves to be useful in practice. Good performances were found for the mtM-HMC (*m*ultiple *t*ime scales *m*ass preconditioned-HMC) compared to the DD-HMC of ref. [163] and to a plain HMC as used in ref. [173]. The algorithm was tested using the standard Wilson gauge action (2.26) and $N_f = 2$ degenerate Wilson fermions (eq. 2.28 with $\mu_{\mathrm{q}} = 0$). The simulations were done on $24^3 \times 32$ lattices with $\beta = 5.6$ and estimated pseudoscalar masses of $m_{\mathrm{PS}} = 665$ MeV, 485 MeV, 380 MeV and 300 MeV (runs *A*, *B*, *C* and *D*). Details of the algorithm parameters as well as results for several quantities such as the plaquette expectation value or the vector mass m_{V} can be found in ref. [167].

The first important observation from this investigation is that for all four aforementioned simulation points the preconditioning masses and time scales can be tuned

	κ	ν [172] (mtM-HMC)	ν [163, 175] (DD-HMC)	ν [173] (HMC)
A	0.15750	0.09(3)	0.69(29)	1.8(8)
B	0.15800	0.11(3)	0.50(17)	5.1(5)
C	0.15825	0.23(9)	0.62(23)	-
D	0.15835	$\simeq 0.35$	0.74(18)	-

Table 2
Comparison of ν values from ref. [172], ref. [163] (with updates from [175] and ref. [173]). The ν-value for simulation point D is only based on an extrapolation of $\tau_{\rm int}(P)$ in $1/m_{\rm PS}^2$.

such that simulations are stable. Examples for Monte Carlo histories of the plaquette expectation value or ΔH can be found in ref. [167].

In order to compare the performance of the mtM-HMC to other HMC variants one could choose two different measures. The first is the *performance figure* $\nu = 10^{-3}(2N_n + 3)\tau_{\rm int}(P)$ as introduced in ref. [163]. $\tau_{\rm int}(P)$ is the integrated autocorrelation time of the plaquette and n is the number of integration steps for the physical operator Q_W^2 necessary for one trajectory. ν represents the number of inversions of the operator Q_W in thousands needed in order to obtain one independent configuration. It is clearly algorithm and machine independent, but it does not account for the preconditioning overhead, which is, at least for the mtM-HMC, not completely negligible. The estimate was that this overhead was roughly a factor of two, and this has been recently confirmed in [174].

The results for the ν-values are summarized in table 2 and, while the ν-values for the mtM-HMC and the DD-HMC are comparable, they are significantly smaller than the values extracted for the plain HMC algorithm used in ref. [173].

Concluding remarks

I have presented an overview of the theoretical properties and numerical results of Wilson twisted mass QCD. To warm up, I started by considering a classical theory with a twisted mass term (tmQCD). In the continuum a twisted mass term can always be rotated away by a non-anomalous change of fermion variables in the functional integral.

On the lattice the twisted mass cannot be rotated away: the standard Wilson lattice action and the Wilson twisted mass (Wtm) lattice action are not related by a change of variables, and as a consequence have different discretization errors. The difference between the two discretizations is governed by the amount of disaglinement, also called twist, in the chiral space between the Wilson term and the mass term. After describing the theoretical properties of Wtm QCD I have shown how the choice of working at full twist, i.e. maximally disaligning the Wilson term and the mass term, is rewarding in many respects. At full twist, the dimension five operators describing the leading discretization errors in physical quantities break chiral symmetry in an "orthogonal" direction respect to the mass term. As a consequence their insertions in correlation functions of multiplicatively renormalizable operators vanish. Physical quantities are then automatically $\mathrm{O}(a)$ improved if we stay at full twist at finite lattice spacing, without the knowledge of any of the improvement coefficients required by the implementation of the Symanzik improvement program. After discussing many technical issues concerning the choice of the critical mass, I have rederived some of the results using the so called physical basis, where the twist is applied to the Wilson term, keeping the mass term in the standard chiral direction.

The disaglinement in chiral space between the mass term and Wilson term causes, at finite lattice spacing, the breaking of isospin and parity symmetry. Both symmetry breakings appear as $\mathrm{O}(a^2)$ cutoff effect. The consequences of the breaking of parity symmetry at finite lattice spacing can be analyzed in the correlation functions with standard techniques. Numerical results seem to indicate that parity breaking cutoff effects are well under control. Isospin breaking cutoff effects induce splittings among flavour multiplets. In particular the neutral and the charged pions are not degenerate at finite lattice spacing, even if they contain degenerate quarks. The splitting is an $\mathrm{O}(a^2)$ effects but numerically not negligible. I have shown that one way to partially mitigate this problem is to use a discretization for the valence quarks which do not break flavour symmetry like the Osterwalder-Seiler action or a Ginsparg-Wilson action. Carefully matching the renormalized quark masses for the valence and the sea quark action, it is then possible to eliminate the isospin splitting at the valence level. At the level of virtual quarks and virtual pions the problem cannot be eliminated, and this is certainly an issue that has to be investigated both theoretically and

numerically in the future. Isospin splitting in other sectors, like in baryon multiplets, seems to be numerically under control.

The O(a^2) cutoff effects of a Wilson-like theory deform the diagram of the chiral phase transition. The chiral phase diagram can be analyzed using a generalization of chiral perturbation theory (χPT) at finite lattice spacing to include the O(a) and O(a^2) cutoff effects. This generalization called W(ilson)χPT predicts two possible scenarios for the chiral phase diagram: the Aoki scenario, the Sharpe-Singleton scenario. There are numerical evidences that close enough to the continuum limit, with a Wilson lattice gauge action and Wtm lattice fermion action the Aoki scenario applies for the quenched model while the Sharpe-Singleton scenario applies for dynamical quarks. A consequence of the Sharpe-Singleton scenario is that even if the twisted mass term gives a sharp infrared cutoff to the lattice theory on each gauge background, there is a minimal value of the twisted mass which can be simulated before encountering a second order phase transition point where the neutral pion is massless. The position of this second order point goes to zero in the continuum as O(a^2) and depends on all the details of the lattice action used. In particular I have shown how using a slightly modified gauge action, like the tree-level Symanzik (tlSym) improved gauge action can mitigate this problem allowing simulations at smaller quark masses given a certain lattice spacing. In particular the tlSym gauge action and the Wtm fermion action allow simulations at a lattice spacing of $a \simeq 0.1$ fm with $M_\pi \simeq 300$ MeV.

A further advantage of Wtm is the possibility to ease the renormalization patterns of phenomenologically relevant physical quantities. The pseudoscalar decay constant, contrary to what happens with Wilson and clover improved fermions, can be computed without the knowledge of any renormalization constant, because at full twist, the decay constant is related to the vector current which is protected from renormalization, because of the exact flavour symmetry of Wtm in the massless limit. Recent results with $N_f = 2$ dynamical simulations show that the chiral behaviour in the pseudoscalar sector can be analyzed very precisely and, within the current understanding of all the systematic effects, it is consistent with NLO χPT. A second example is the provided by B_K which parametrizes the non-perturbative contribution to the indirect CP violation in the kaon sector. Two different strategies have been presented which remove the mixing of the relevant four-fermion operator, both based on the observation that B_K can be evaluated also from a parity violating four fermion operator which renormalizes multiplicatively and can be extracted using twisted mass regularizations.

I have concluded, in the last section, with a brief digression on recent algorithmic developments to simulate dynamical Wilson-like fermions.

Wtm can be used to describe also non-degenerate quarks. I have discussed two different discretizations which describe non-degenerate quarks in the context of tm

QCD. First results with *up*, *down*, *strange* and *charm* dynamical quarks show that simulations of realistic QCD with realistic physical parameters are within reach of the current machines and algorithms.

Although presently not all aspects of Wtm are fully investigated, Wtm is a powerful discretization of lattice QCD, and it certainly belongs to the pool of well founded fermion actions that ought to be used to control the continuum limit of physical quantities of interest.

I hope that the ongoing theoretical and numerical investigations related to Wtm might help in the quest for solving QCD.

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A Definitions and conventions

A.1 Index conventions

Lorentz indices are taken from the middle Greek alphabet $\mu, \nu, \ldots$ and run from 0 to 3. Latin indices k, l, ... are used to label the components of the spatial vectors and run from 1 to 3. For Dirac indices we use letters α, β, ... from the beginning of the Greek alphabet and they run from 1 to 4. Colour vectors in the fundamental representation of SU(N_c) carry indices A,B, ... ranging from 1 to N_c, while for vectors in the adjoint representation capital letters a, b, ... running from 1 to $N_\mathrm{c}^2 - 1$ are employed. By abuse of notation for flavour vectors in the fundamental representation of SU(N_f) we use latin indices i,j,... ranging from 1 to N_f while for vectors in the adjoint representation indices a,b,... running from 1 to $N_\mathrm{f}^2 - 1$ are used. It will be clear from the context to which case we are refering to. Repeated indices are always summed over unless stated and scalar products are taken with euclidean metric.

A.2 Dirac matrices

We choose a chiral representation for the Dirac matrices, where

$$\gamma_\mu = \begin{pmatrix} 0 & e_\mu \\ e_\mu^\dagger & 0 \end{pmatrix}.$$

The 2×2 matrices e_μ are taken to be

$$e_0 = -1, \qquad e_k = -i\sigma_k, \tag{A.1}$$

with σ_k the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

It is then easy to check that

$$\gamma_\mu = \gamma_\mu^\dagger, \qquad \{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}. \tag{A.2}$$

Furthermore we define

$$\gamma_5 = \gamma_0\gamma_1\gamma_2\gamma_3 \qquad \Rightarrow \qquad \gamma_5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In particular

$$\gamma_5 = \gamma_5^\dagger, \qquad \gamma_5^2 = 1, \tag{A.3}$$

and the hermitian matrices

$$\sigma_{\mu\nu} = \frac{i}{2}[\gamma_\mu, \gamma_\nu], \qquad \sigma_{\mu\nu} = \sigma_{\mu\nu}^\dagger, \tag{A.4}$$

are explicitly given by

$$\sigma_{0k} = \begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix}, \qquad \sigma_{ij} = -\epsilon_{ijk} \begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix},$$

where ϵ_{ijk} is the totally antisymmetric tensor with $\epsilon_{123} = 1$.

A.3 Gauge group

A representation of the Lie algebra of SU(N_c) is given by complex $N_\mathrm{c} \times N_\mathrm{c}$ matrices X_{AB} which satisfy

$$X^\dagger = -X, \qquad \mathrm{tr}\{X\} = X_{AA} = 0. \tag{A.5}$$

It is possible to choose a basis in this matrix space T^a, $a = 1,2,\ldots N_\mathrm{c}^2 - 1$ that satisfies

$$\mathrm{tr}\{T^a T^b\} = -\frac{1}{2}\delta^{ab}. \tag{A.6}$$

For $N_\mathrm{c} = 3$ the standard basis is

$$T^a = \frac{\lambda^a}{2i}, \qquad a = 1, \ldots 8, \tag{A.7}$$

where λ^a denote the Gell-Mann matrices. With this convention the structure constants f^{abc}, defined by

$$[T^a, T^b] = f^{abc} T^c, \tag{A.8}$$

are real and totally antisymmetric.

A.4 Lattice derivatives

Ordinary lattice forward and backward derivatives are diagonal in colour space and are defined by

$$\partial_\mu f(x) = \frac{1}{a}[f(x + a\hat{\mu}) - f(x)], \tag{A.9}$$

$$\partial_\mu^* f(x) = \frac{1}{a}[f(x) - f(x - a\hat{\mu})], \tag{A.10}$$

where $\hat{\mu}$ denotes the unit vector in direction μ. The gauge covariant derivatives acting on a quark fields are not trivial anymore in colour space and they are defined by

$$\nabla_\mu \chi(x) = \frac{1}{a}[U(x,\mu)\chi(x+a\hat{\mu}) - \chi(x)], \tag{A.11}$$

$$\nabla^*_\mu \chi(x) = \frac{1}{a}[\chi(x) - U(x-a\hat{\mu},\mu)^{-1}\chi(x-a\hat{\mu})]. \tag{A.12}$$

The left action of the lattice derivative operators is defined by

$$\overline{\chi}(x)\overleftarrow{\nabla}_\mu = \frac{1}{a}[\overline{\chi}(x+a\hat{\mu})U(x,\mu)^{-1} - \overline{\chi}(x)], \tag{A.13}$$

$$\overline{\chi}(x)\overleftarrow{\nabla}^*_\mu = \frac{1}{a}[\overline{\chi}(x) - \overline{\chi}(x-a\hat{\mu})U(x-a\hat{\mu},\mu)]. \tag{A.14}$$

A.5 Continuum gauge fields

The gauge field in a continuum gauge theory belongs to the algebra of the gauge group and may be written as

$$G_\mu(x) = G^a_\mu(x)T^a \tag{A.15}$$

with real components $G^a_\mu(x)$. The field strength tensor

$$F_{\mu\nu} = \partial_\mu G_\nu(x) - \partial_\nu G_\mu(x) + [G_\mu(x), G_\nu(x)], \tag{A.16}$$

can be also decomposed in the same way. The right and left covariant derivatives are defined by

$$D_\mu \chi(x) = (\partial_\mu + G_\mu)\chi(x) \tag{A.17}$$

$$\overline{\chi}(x)\overleftarrow{D}_\mu = \overline{\chi}(x)(\overleftarrow{\partial}_\mu - G_\mu). \tag{A.18}$$

We stress that ∂_μ in formulæ(A.17,A.18) are continuum partial derivatives, and do not have to be confused with the lattice derivative (A.9).

B Symmetries in the twisted basis

We list here the form of the relevant symmetries for a generic angle ω. The $SU(2)$ axial and vector twisted transformations take the form

$$SU_{\rm V}(2)_\omega: \begin{cases} \chi(x) \longrightarrow \exp(-i\frac{\omega}{2}\gamma_5\tau^3)\exp(i\frac{\alpha^a_V}{2}\tau^a)\exp(i\frac{\omega}{2}\gamma_5\tau^3)\chi(x), \\ \overline{\chi}(x) \longrightarrow \overline{\chi}(x)\exp(i\frac{\omega}{2}\gamma_5\tau^3)\exp(-i\frac{\alpha^a_V}{2}\tau^a)\exp(-i\frac{\omega}{2}\gamma_5\tau^3). \end{cases} \tag{B.1}$$

$$SU_{\rm A}(2)_\omega\colon \begin{cases}\chi(x) \longrightarrow \exp(-i\frac{\omega}{2}\gamma_5\tau^3)\exp(i\frac{\alpha_A^a}{2}\gamma_5\tau^a)\exp(i\frac{\omega}{2}\gamma_5\tau^3)\chi(x),\\ \overline{\chi}(x) \longrightarrow \overline{\chi}(x)\exp(i\frac{\omega}{2}\gamma_5\tau^3)\exp(i\frac{\alpha_A^a}{2}\gamma_5\tau^a)\exp(-i\frac{\omega}{2}\gamma_5\tau^3).\end{cases} \tag{B.2}$$

The twisted discrete symmetries that involve axis reflections (parity and time reversal), using the gamma matrix representation given above, are

$$\mathcal{P}_\omega\colon \begin{cases}U(x_0,\mathbf{x};0) \longrightarrow U(x_0,-\mathbf{x};0), \quad U(x_0,\mathbf{x};k) \longrightarrow U^{-1}(x_0,-\mathbf{x}-a\hat{k};k), \quad k=1,2,3\\ \chi(x_0,\mathbf{x}) \longrightarrow \gamma_0\exp(i\omega\gamma_5\tau^3)\chi(x_0,-\mathbf{x}),\\ \overline{\chi}(x_0,\mathbf{x}) \longrightarrow \overline{\chi}(x_0,-\mathbf{x})\exp(i\omega\gamma_5\tau^3)\gamma_0,\end{cases} \tag{B.3}$$

$$\mathcal{T}_\omega\colon \begin{cases}U(x_0,\mathbf{x};0) \longrightarrow U^{-1}(-x_0-a,\mathbf{x};0), \quad U(x_0,\mathbf{x};k) \longrightarrow U(-x_0,\mathbf{x};k), \quad k=1,2,3\\ \chi(x_0,\mathbf{x}) \longrightarrow i\gamma_0\gamma_5\exp(i\omega\gamma_5\tau^3)\chi(-x_0,\mathbf{x}),\\ \overline{\chi}(x_0,\mathbf{x}) \longrightarrow -i\overline{\chi}(-x_0,\mathbf{x})\exp(i\omega\gamma_5\tau^3)\gamma_5\gamma_0.\end{cases} \tag{B.4}$$

Charge conjugation takes a form that is invariant under the change of variables (2.6)

$$\mathcal{C}\colon \begin{cases}U(x;\mu) \longrightarrow U(x;\mu)^*,\\ \chi(x) \longrightarrow C^{-1}\overline{\chi}(x)^T,\\ \overline{\chi}(x) \longrightarrow -\chi(x)^T C,\end{cases} \tag{B.5}$$

where C satisfies

$$-\gamma_\mu^T = C\gamma_\mu C^{-1}, \qquad \gamma_5 = C\gamma_5 C^{-1}. \tag{B.6}$$

In the chosen gamma matrix representation a possible choice is $C = i\gamma_0\gamma_2$ so that $C = C^\dagger = C^{-1}$.

C Transfer matrix

We use here the original notation of ref. [28]. The transfer matrix as an operator in Fock space and as an integral kernel with respect to the gauge fields has the structure

$$T_0[U,U'] = \hat{T}_{\rm F}^\dagger(U)K_0[U,U']\hat{T}_{\rm F}(U'), \tag{C.1}$$

with pure gauge kernel K_0 and the fermionic part

$$\hat{T}_{\rm F}(U) = \det(2\kappa B)^{1/4}\exp(\hat{\eta}^\dagger P_- C\hat{\eta})\exp(-\hat{\eta}^\dagger\gamma_0 M\hat{\eta}). \tag{C.2}$$

Here, the operators $\hat{\eta}_i(\mathbf{x})$ are canonical (i is a shorthand for colour, spin and flavour indices)

$$\{\hat{\eta}_i(\mathbf{x}),\hat{\eta}_j^\dagger(\mathbf{y})\} = \delta_{ij}a^{-3}\delta_{\mathbf{xy}}, \tag{C.3}$$

and B and C are matrix representations of the difference operators

$$B(\mathbf{x},\mathbf{y})_{A\alpha;B\beta} = \delta_{\alpha\beta}\Big\{\delta_{AB}\delta(\mathbf{x},\mathbf{y}) - \kappa\sum_{k=1}^{3}\Big[U(\mathbf{x};k)_{AB}\delta(\mathbf{x}+a\hat{k},\mathbf{y}) + U(\mathbf{y};k)^{-1}_{AB}\delta(\mathbf{y}+a\hat{k},\mathbf{x})\Big]\Big\} \tag{C.4}$$

$$C(\mathbf{x},\mathbf{y})_{A\alpha;B\beta} = \sum_{k=1}^{3}(\gamma_k)_{\alpha\beta}\frac{1}{2}\Big[U(\mathbf{x};k)_{AB}\delta(\mathbf{x}+a\hat{k},\mathbf{y}) - U(\mathbf{y};k)^{-1}_{AB}\delta(\mathbf{y}+a\hat{k},\mathbf{x})\Big] \tag{C.5}$$

The matrix M is defined as

$$M = \frac{1}{2}\ln\left(\frac{1}{2\kappa}B\right), \tag{C.6}$$

In order to prove the positivity of the transfer matrix it is enough to show that $\hat{T}_{\mathrm{F}}$ is bounded and invertible and that $K_0[U,U']$ is positive. $K_0[U,U']$ depends only on the gauge action and the proof of its positivity for the Wilson gauge action can be found in [28]. What remains to be proven is the positivity of B. Let's indicate with $\hat{\mathcal{U}}_i$ the following unitary operator

$$\hat{\mathcal{U}}_i(\psi)(x) = U_i(x)\psi(x+a\hat{i}) \tag{C.7}$$

then the operator whose kernel is B (C.12) can be written as

$$\hat{B} = 1 - \kappa\sum_{i=1}^{3}\Big[\hat{\mathcal{U}}_i + \hat{\mathcal{U}}_i^{\dagger}\Big] \tag{C.8}$$

We can then write the eigenvalues of this matrix in the following way

$$\lambda(\hat{B}) = 1 - \kappa\sum_{i=1}^{3}\Big[2\mathbb{R}\mathrm{e}\,\lambda(\hat{\mathcal{U}}_i)\Big] \tag{C.9}$$

and given the unitarity of $\hat{\mathcal{U}}_i$ we can conclude

$$1 - 6\kappa \leq \lambda(\hat{B}) \leq 1 + 6\kappa \tag{C.10}$$

From this we can conclude that if $|\kappa| < \frac{1}{6}$ then the operator B is positive definite.

We remark here that in principle physical positivity can be violated at finite lattice spacing, but one should have available a clean definition of the transfer matrix and the corresponding eigenvalues. Moreover positivity should be lost only at the cutoff scale, in order to become unimportant in the continuum limit. In ref. [176] it has been shown indeed that this is the case for improved gauge actions.

In ref. [29] it was shown that Wtm for degenerate quarks has also a well defined and positive tranfer matrix. The twisted mass term can be added to the antihermitian C matrix without changing the given proof

$$C_{\rm Wtm}(\mathbf{x},\mathbf{y})_{A\alpha i;B\beta j} = \delta_{ij}\sum_{k=1}^{3}(\gamma_k)_{\alpha\beta}\frac{1}{2}\Big[U(\mathbf{x};k)_{AB}\delta(\mathbf{x}+a\hat{k},\mathbf{y}) - U(\mathbf{y};k)^{-1}_{AB}\delta(\mathbf{y}+a\hat{k},\mathbf{x})\Big] + ia\mu_{\rm q}(\gamma_5)_{\alpha\beta}(\tau^3)_{ij}\delta_{AB}\ , \tag{C.11}$$

except that $\mu_{\rm q}$ must be real.

But if we want to add a twisted term for non-degenerate quarks as given in eq. (3.20) one needs to add this to the hermitian matrix B. To keep the matrix B positive the constraint on the values of κ has to be changed In fact the matrix B is given now by

$$\delta_{\alpha\beta}\Big\{\delta_{AB}\delta(\mathbf{x},\mathbf{y})\Big[1+2\kappa a\epsilon_{\rm q}\tau^1\Big]_{ij} - \delta_{ij}\kappa\sum_{k=1}^{3}\Big[U(\mathbf{x};k)_{AB}\delta(\mathbf{x}+a\hat{k},\mathbf{y}) + U(\mathbf{y};k)^{-1}_{AB}\delta(\mathbf{y}+a\hat{k},\mathbf{x})\Big]\Big\}\ . \tag{C.12}$$

Repeating the same argument given in eqs. (C.8- C.10) we obtain the new constraint

$$|\kappa| < \frac{1}{6+2a\epsilon_{\rm q}}, \qquad \epsilon_{\rm q} > 0. \tag{C.13}$$

D O(a) improvement

In this appendix we give more technical details of the dimension 5 operators describing the O(a) effects of the Wtm lattice action. In sect. 2 we have analyzed the form of the continuum action S_0 using the symmetries of the lattice theory.

We now construct S_1 in eq. (4.3), which contains dimension five operators. To classify all the possible operators, we have to use again the symmetries of the lattice action, and make use of partial integration in (4.5) given the space integration over y. As for S_0 the residual $U_{\rm V}(1)_3$ flavour symmetry forbids bilinears with $\tau^{1,2}$. A number of potential terms can be excluded by the $\tilde{P} = P \times (\mu_{\rm q} \to -\mu_{\rm q})$ symmetry, because it implies that parity violating dimension 5 fields have to be multiplied with a twisted mass term to an odd power. We can exclude then terms like $m_{\rm q}\mu_{\rm q}\overline{\chi}\chi$, $m_{\rm q}^2\overline{\chi}i\gamma_5\tau_3\chi$, $\mu_{\rm q}^2\overline{\chi}i\gamma_5\tau_3\chi$, $\overline{\chi}D^2i\gamma_5\tau_3\chi$ and $\overline{\chi}i\sigma_{\mu\nu}F_{\mu\nu}i\gamma_5\tau_3\chi$. The last of these, the "twisted Pauli term", requires a factor of $\mu_{\rm q}$ and thus appears only in S_2. Charge conjugation symmetry excludes a term like $i\mu_{\rm q}\{\overline{\chi}\gamma_5\tau^3\gamma_\mu\overrightarrow{D}_\mu\chi + \overline{\chi}\overleftarrow{D}_\mu\gamma_\mu\gamma_5\tau^3\chi\}$.

The list of the possible fields contributing to $\mathcal{L}_1(y)$ then is [9, 29]

$$\mathcal{O}_1 = i\overline{\chi}\sigma_{\mu\nu}F_{\mu\nu}\chi, \tag{D.1}$$

$$\mathcal{O}_2 = m_{\rm q}{\rm tr}\{F_{\mu\nu}F_{\mu\nu}\}, \tag{D.2}$$
$$\mathcal{O}_3 = m_{\rm q}^2\overline{\chi}\chi, \tag{D.3}$$
$$\mathcal{O}_4 = m_{\rm q}\mu_{\rm q}i\overline{\chi}\gamma_5\tau^3\chi, \tag{D.4}$$
$$\mathcal{O}_5 = \mu_{\rm q}^2\overline{\chi}\chi, \tag{D.5}$$
$$\mathcal{O}_6 = m_{\rm q}\{\overline{\chi}\gamma_\mu\overrightarrow{D}_\mu\chi - \overline{\chi}\overleftarrow{D}_\mu\gamma_\mu\chi\}, \tag{D.6}$$
$$\mathcal{O}_7 = \{\overline{\chi}\overrightarrow{D}_\mu\overrightarrow{D}_\mu\chi + \overline{\chi}\overleftarrow{D}_\mu\overleftarrow{D}_\mu\chi\}. \tag{D.7}$$

To apply the Symanzik improvement program one needs to improve also the local fields in the correlation functions. To be concrete we give here the example of the currents A_μ^a, V_μ^a and P^a which appear in the Ward identities (2.18,2.19). The local operators contributing to the leading correction term in the effective axial current A_μ^a are [9, 10, 29]:

$$(\mathcal{O}_8)_\mu^a = \overline{\chi}\gamma_5\frac{\tau^a}{2}\sigma_{\mu\nu}\overrightarrow{D}_\nu\chi - \overline{\chi}\overleftarrow{D}_\nu\sigma_{\mu\nu}\gamma_5\frac{\tau^a}{2}\chi, \tag{D.8}$$

$$(\mathcal{O}_9)_\mu^a = \overline{\chi}\gamma_5\frac{\tau^a}{2}\overrightarrow{D}_\mu\chi + \overline{\chi}\overleftarrow{D}_\mu\gamma_5\frac{\tau^a}{2}\chi, \tag{D.9}$$

$$(\mathcal{O}_{10})_\mu^a = m_{\rm q}\overline{\chi}\gamma_\mu\gamma_5\frac{\tau^a}{2}\chi, \tag{D.10}$$

$$(\mathcal{O}_{11})_\mu^a = \mu_{\rm q}\epsilon^{3ab}\overline{\chi}\gamma_\mu\frac{\tau^b}{2}\chi\ , \tag{D.11}$$

for the pseudoscalar density P^a we need

$$(\mathcal{O}_{12})^a = m_{\rm q}\overline{\chi}\gamma_5\frac{\tau^a}{2}\chi\ , \tag{D.12}$$

and for the vector current V_μ^a

$$(\mathcal{O}_{13})_\mu^a = \overline{\chi}\sigma_{\mu\nu}\frac{\tau^a}{2}\overrightarrow{D}_\nu\chi + \overline{\chi}\overleftarrow{D}_\nu\sigma_{\mu\nu}\frac{\tau^a}{2}\chi, \tag{D.13}$$

$$(\mathcal{O}_{14})_\mu^a = m_{\rm q}\overline{\chi}\gamma_\mu\frac{\tau^a}{2}\chi, \tag{D.14}$$

$$(\mathcal{O}_{15})_\mu^a = \mu_{\rm q}\epsilon^{3ab}\overline{\chi}\gamma_\mu\gamma_5\frac{\tau^b}{2}\chi\ . \tag{D.15}$$

In general we consider a generic connected lattice correlation function $\langle\Phi\rangle$ (4.7) at $x_1 \neq x_2 \neq \cdots \neq x_n$. In the effective theory up to order a, $\langle\Phi\rangle$ is given by eq. (4.8). Without contact terms the continuum equation of motions can be used in order to constrain the set of operators $\mathcal{O}_i$. Since we consider correlation functions with $x_1 \neq x_2 \neq \cdots \neq x_n$, the only contact terms arise when the argument y of $\mathcal{L}_1(y)$

is equal to the argument x_k of one of the fields in the correlation function. But as we have discussed in sect. 4.1 this simply amounts to a redefinition of ϕ_1, so the equations of motion of the continuum theory can be used to simplify the field basis for the effective action and operators. But it is important to remember that the coefficients appearing in the linear combination ϕ_1 will depend on the choice of the basis and on the value of the coefficients of $\mathcal{L}_1$.

The list of operators given above for the O(a) lattice correction can then be reduced using the field equations. Formal application of the field equations gives

$$\mathcal{O}_1 - \mathcal{O}_7 + 2\mathcal{O}_5 + 2\mathcal{O}_3 = 0 \tag{D.16}$$

$$\mathcal{O}_6 + 2\mathcal{O}_3 + 2\mathcal{O}_4 = 0, \tag{D.17}$$

which allows to eleminate $\mathcal{O}_6$ and $\mathcal{O}_7$.

A technical remark has to be made here. The naive relations (D.16,D.17) are obtained at tree-level of perturbation theory. At higher order they should be replaced by linear combinations of all basis elements with coefficients that depend on the coupling. Nevertheless the simple existence of such relations allows us to eliminate $\mathcal{O}_6$ and $\mathcal{O}_7$.

The same procedure can be adopted to eliminate redundant terms for the operators describing the leading O(a) corrections to the pseudoscalar density and the axial and vector current, similarly to what we have done for the operators contributing to the effective action,

For example for the axial current the operator $(\mathcal{O}_8)^a_\mu$ can be eliminated using the equations of motion.

E Automatic O(a) improvement

In this appendix we will give the basic idea of the first proof of automatic O(a) improvement [11]. We do not give the whole proof and we invite the reader to look at the original paper [11] for more details.

The form of the unimproved lattice action is $S = S_G + S_F$ and the Wtm quark action S_F is defined in eq. (2.28). The form of the gauge action is not relevant because it has leading O(a^2) discretization errors. A general Symanzik expansion of a connected lattice correlation function (4.8) of multiplicatively renormalized fields contains coefficients (e.g. in the linear combinations which define $\mathcal{L}_1$) that will depend on the bare parameters of the lattice action.

We consider first the plain Wilson action setting $\mu_{\rm q} = 0$ in eq. (2.28), and we define here the discrete axial-vector transformation [24]

$$\mathcal{R}_5 : \begin{cases} \chi(x_0, \mathbf{x}) \to \gamma_5 \chi(x_0, \mathbf{x}) \\ \overline{\chi}(x_0, \mathbf{x}) \to -\overline{\chi}(x_0, \mathbf{x})\gamma_5 \end{cases} \tag{E.1}$$

The lattice action is invariant if after a $\mathcal{R}_5$ transformation on the fields we change also the sign of the Wilson term and the mass term. In particular the lattice action (2.28), with $\mu_{\rm q} = 0$, is invariant under the following transformation

$$\mathcal{R}_5^{\rm sp} \equiv \mathcal{R}_5 \times [r \to -r] \times [m_0 \to -m_0]. \tag{E.2}$$

This happens because both Wilson and mass terms are odd under the $\mathcal{R}_5$ symmetry. It is also interesting to note that both the Wilson and the mass term have odd dimensions, if we exclude the bare quark mass m_0 and the lattice spacing a in the counting. As a consequence of this, all the terms of $\mathrm{O}(a)$ in the Symanzik expansion (4.8) will have opposite definite properties under $r \to -r$, such that averages of correlation functions computed on the lattice with opposite values of r have a faster approach to the continuum limit, i.e. the $\mathrm{O}(a)$ effects are cancelled [25] .

If the theory is tuned to full twist, $\omega = \pi/2$, this averaging procedure is automatic. In fact if we consider the action (5.2) the transformation $r \to -r$ is equivalent to $\omega \to \omega + \pi$.

F Nucleon operators in the twisted basis

In this appendix we show how the nucleon operators change in the twisted basis. This is a rather simple exercise and it is shown here just as an example how to proceed in a general case. The starting point is the lattice action in eq. (2.28). The connection between correlators in standard QCD and tmQCD can be inferred from classical consideration. We consider the doublet

$$\chi = \begin{pmatrix} u \\ \\ d \end{pmatrix}.$$

The axial rotation in eq. (2.6) for single flavour takes the form

$$u(x) \to \exp\Big(i\frac{\omega}{2}\gamma_5\Big)u(x) \tag{F.1}$$

[24] This transformation is not anomalous since is the product of 2 non-anomalous vector and axial transformations in the same isospin direction.
[25] Ideas in this direction were already put forward in [12, 177].

$$d(x) \to \exp\Big(-i\frac{\omega}{2}\gamma_5\Big)d(x) \tag{F.2}$$

and the corresponding for the antiquark fields. The proton field

$$\mathscr{P} = u_A[u_B^T C^{-1}\gamma_5 d_C]\epsilon_{ABC}, \tag{F.3}$$

transforms in

$$\mathscr{P} \to \exp\left(i\frac{\omega}{2}\gamma_5\right)\mathscr{P}. \tag{F.4}$$

In QCD the proton correlation function

$$G_{\mathscr{P}}(x_0) = \int \mathrm{d}^3x \langle \mathscr{P}(x_0,\mathbf{x})\bar{\mathscr{P}}(0,\mathbf{0})\rangle_{\mathrm{QCD}}, \tag{F.5}$$

has the general decomposition (for simplicity we consider only the leading exponential contributions)

$$\begin{aligned} G_{\mathscr{P}}(x_0) = {} & P_+\theta(x_0)A_{\mathscr{P}^+}e^{-M_{\mathscr{P}^+}x_0} + P_-\theta(-x_0)A_{\mathscr{P}^+}e^{M_{\mathscr{P}^+}x_0} - \\ & P_+\theta(-x_0)A_{\mathscr{P}^-}e^{M_{\mathscr{P}^-}x_0} - P_-\theta(x_0)A_{\mathscr{P}^-}e^{-M_{\mathscr{P}^-}x_0}, \end{aligned} \tag{F.6}$$

where

$$P_\pm = \frac{1}{2}\left(1 \pm \gamma_0\right). \tag{F.7}$$

The backward propagating contributions correspond to the antiparticles of the forward propagating states with opposite parity. The desired state is obtained using the appropriate projection operator $P_\pm$ and the appropriate direction of propagation. Given the classical correspondence between QCD and tmQCD (2.23) the mass of the desired state in the proton channel can be extracted from the exponential behaviour of the following correlator in tm QCD

$$\mathrm{Tr}\left[P_\pm G^{tm}_{\mathscr{P}}(x_0)\right] \tag{F.8}$$

where

$$G^{tm}_{\mathscr{P}}(x_0) = \int \mathrm{d}^3x \left\langle e^{\left(i\frac{\omega}{2}\gamma_5\right)}\mathscr{P}(x_0,\mathbf{x})\bar{\mathscr{P}}(0,\mathbf{0})e^{\left(i\frac{\omega}{2}\gamma_5\right)}\right\rangle_{\mathrm{tmQCD}}. \tag{F.9}$$

The correlation function in eq. (F.9) can now be computed on the lattice with the Wtm lattice action (2.28).

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