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Continuum Limit of Overlap Valence Quarks on a Twisted Mass Sea

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Abstract

We study a lattice QCD mixed action with overlap valence quarks on two flavours of Wilson maximally twisted mass sea quarks. Employing three different matching conditions to relate both actions to each other, we investigate the continuum limit by using three values of the lattice spacing ranging from $a \approx 0.05$ fm to 0.08 fm. A particular emphasis is put on the effect on physical observables of the topological zero modes appearing in the valence overlap operator. We estimate the region of parameter space where the contribution from these zero modes is sufficiently small such that their effects can be safely controlled and a restoration of unitarity of the mixed action in the continuum limit is reached.

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1 Introduction

The discretization of the QCD action on a lattice provides a framework for a quantitative description of the non-perturbative phenomena inherent to hadronic physics at low energies. The way of discretizing the continuum QCD action is, however, by no means unique and leaves a large number of choices. Although all lattice actions used in practise respect the principle of local gauge

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invariance, they often break a number of continuum symmetries depending on the particular choice of the lattice action used. A most notable example is the explicit breaking of chiral symmetry on the lattice in order to avoid unwanted additional fermion excitations, the so-called doublers [1–3]. There exist, however, lattice fermion actions which are constructed from Dirac operators that satisfy the Ginsparg-Wilson relation [4] and lead to an exactly preserved but lattice modified chiral symmetry [5]. The big disadvantage of these Ginsparg-Wilson type fermions is that they are computationally very expensive.

A possible way to restore a desired symmetry –at least partially, since it will not by respected by the sea quark action – is the approach of so-called mixed actions, corresponding to the use of different discretizations of the Dirac operator in the valence and sea sectors. Of course, using such a mixed action it needs to be guaranteed that a well defined continuum limit, which corresponds to the universality class of continuum QCD, is reached eventually. This can be achieved by imposing an appropriate matching condition relating both actions to each other and which fixes the physical situation at each value of a non-zero lattice spacing. Hence, a well defined continuum limit can be reached.

Although in this way mixed actions offer an advantage since the valence quarks can have improved symmetry properties with respect to the sea quark action, they also provide challenges. Even when imposing a matching condition, the sea quark and valence quark theories are not fully matched and differ by discretization effects, which lead to unitarity violations in physical quantities. It is therefore an important question to understand the characteristics of a mixed action approach and to learn how and whether indeed the correct continuum limit is reached. In particular, it is an interesting and important question, whether and how the inherent mismatch of the eigenvalue spectra affect physical observables and influence possibly the continuum limit.

It is the goal of this work to address the above questions by studying a particular mixed action setup, employing maximally twisted mass (MTM) fermions [6, 7] in the sea and chirally invariant overlap fermions [8, 9] in the valence sector. As anticipated above, the mismatch of the spectra of the lattice Dirac operators employed in the sea and the valence actions will be a particular concern. While the overlap Dirac operator exhibits exact chiral zero modes, for any non-zero value of the lattice spacing, the twisted mass Dirac operator does not, at least at lattice spacings used in this work. As discussed already in ref. [10], the quantitative effects of these unmatched zero modes on physical observables will depend on the quark mass and the physical volume used in the numerical simulation.

We will investigate the mesonic sector of the theory and study the continuum limit of light pseudoscalar meson observables by using three values of the lattice spacing ranging from $a \approx 0.05\,\mathrm{fm}$ to $0.08\,\mathrm{fm}$ at a fixed lattice

size of $L \approx 1.3\,\mathrm{fm}$, and quark masses $m_q^{\overline{\mathrm{MS}}}(\mu = 2\,\mathrm{GeV}) \approx 20\,\mathrm{MeV}$ and $m_q^{\overline{\mathrm{MS}}}(\mu = 2\,\mathrm{GeV}) \approx 40\,\mathrm{MeV}$. These values of the quark masses correspond to infinite volume pseudoscalar masses of approximately 300 MeV and 450 MeV, respectively. We also study finite size effects by considering three values of the lattice size between $L \approx 1.3\,\mathrm{fm}$ and $2.0\,\mathrm{fm}$. The choice of this parameter region (quark mass, lattice size and lattice spacing) allows us to perform then a systematic study of our mixed action setup.

Mixed actions are currently being used by various groups. In the case of valence overlap quarks, studies using domain wall sea fermions [11,12] or Wilson clover sea quarks [13, 14] have been carried out. Domain wall valence fermions on staggered sea quarks have also been extensively used [15–17]. Mixed actions in which variants of the sea action are used in the valence sector, such as Osterwalder-Seiler fermions on a twisted mass sea, have also been recently studied [18–20]. The extension of chiral perturbation theory to the context of mixed actions [21–23] provides a useful analytic control of the light quark mass dependence of several physical quantities in the regime of parameters (quark mass, lattice size and lattice spacing) where the effective theory can be applied.

As said above, in this paper, we perform a systematic study of a mixed action with overlap valence fermions on a Wilson twisted mass sea, by focusing on light pseudoscalar meson observables. In Section 2 we introduce the mixed action setup by shortly reviewing the overlap and twisted mass formalisms and introducing the quark mass matching procedure, which is illustrated in the free theory. Section 3 describes the simulation setup and Section 4 presents the results of the continuum limit study of the mixed action for our light quark mass ensembles. Section 5 provides an interpretation and discussion of the results. In Section 6 we discuss the regime of heavier quark masses and finite size effects. Section 7 concludes and provides an estimate of the regime of parameters where the contribution in the valence sector of the topological zero modes on physical observables is small enough such that a proper control of the restoration of unitarity of the mixed action becomes possible.

2 Mixed Action: Fermionic Actions, Matching and Illustration in the Free Theory

2.1 Overlap Fermions

Overlap fermions were introduced in 1997 by Neuberger [8, 9], who found a particularly simple form of a lattice Dirac operator that obeys the Ginsparg-Wilson relation [4]. This implies that overlap (ov) fermions preserve a lattice

version of chiral symmetry at any value of the lattice spacing [5]. The massless overlap Dirac operator is given by [1]:

$$\hat{D}_{\rm ov}(0) = \frac{1}{a}\Big(1 - A(A^\dagger A)^{-1/2}\Big). \tag{1}$$

The kernel operator A reads:

$$A = 1 + s - a\hat{D}_{\rm Wilson}(0), \tag{2}$$

where s is a parameter which satisfies $|s| < 1$. The Wilson-Dirac operator is defined by:

$$\hat{D}_{\rm Wilson}(m_0) = \frac{1}{2}\left(\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a\nabla^*_\mu\nabla_\mu\right) + m_0, \tag{3}$$

where m_0 is the bare Wilson quark mass and ∇_μ, ∇^*_μ are the forward and backward covariant derivatives, respectively. The massive overlap Dirac operator is given by:

$$\hat{D}_{\rm ov}(m_{\rm ov}) = \left(1 - \frac{am_{\rm ov}}{2}\right)\hat{D}_{\rm ov}(0) + m_{\rm ov},$$

where $m_{\rm ov}$ is the bare overlap quark mass. Note that despite the appearance of the square root in eq. (1), the overlap operator is local in the sense of exponentially decaying coupling strengths as a function of the distance between lattice points [25].

Operators preserving the Ginsparg-Wilson relation develop topological zero modes and fulfil the index theorem at finite lattice spacing [26]. Moreover, chiral symmetry allows to improve the theory at $\mathcal{O}(a)$. Indeed, observables computed with overlap fermions are not affected by $\mathcal{O}(a)$ lattice artefacts, provided that $\mathcal{O}(a)$-improved interpolating operators are used (see e.g. [27]).

The overlap quark mass $m_{\rm ov}$ renormalizes multiplicatively with a renormalisation factor $Z_m = 1/Z_{\rm P}$, where P stands for the pseudoscalar density. The decay constant f_π of a mass degenerate pseudoscalar meson, carrying a mass m_π, can be determined by means of the two-point pseudoscalar correlation function $C_{\rm PP}(t)$ via the following expression:

$$f_\pi^{\rm ov} = \frac{2m_{\rm ov}}{(m_\pi^{\rm ov})^2}\,|\langle 0|P|\pi\rangle_{\rm ov}|\,.$$

It is known that in practise, overlap fermions are demanding from the computational point of view. With respect to Wilson type fermions the overall cost can grow by one to two orders of magnitude [2]. Moreover, the discontinuities

[1] For a review about overlap fermions, see e.g. [24].

[2] We refer to [28] for a detailed comparison to Wilson twisted mass fermions.

of the overlap operator while changing topological sectors pose a problem to the standard Molecular Dynamics algorithm used in dynamical quark simulations. Modifications of the Molecular Dynamics evolution to tackle this problem [29–32] imply a further significant increase in the computational cost. A way to avoid the discontinuity problem is to modify the action in such a way that the topological charge remains fixed [33,34]. However, this procedure introduces additional $\mathcal{O}(1/V)$ finite volume effects which need to be taken into account in the determination of physical observables.

2.2 Wilson Twisted Mass Fermions

Twisted mass (tm) fermions [6] are defined by adding a chirally rotated mass term to the Wilson-Dirac operator in eq. (3) as follows:

$$\hat{D}_{\rm tm} = \hat{D}_{\rm Wilson}(m_0) + i\mu_q\gamma_5\tau_3 \,, \tag{4}$$

where μ_q is the twisted mass parameter and τ_3 is the third Pauli matrix acting in flavour space.

Wilson twisted mass fermions were introduced to address the problem of unphysically small eigenvalues of the Wilson-Dirac operator [6]. Furthermore, by tuning the mass m_0 to its critical value $m_{\rm crit}$, a situation denoted by maximal twist, physical observables are automatically $\mathcal{O}(a)$ improved [7] independently of the operator which is considered, implying that no additional, operator specific improvement coefficients need to be computed. Detailed studies of the continuum-limit scaling in the quenched approximation [35] and with two dynamical quarks [36] have demonstrated that, after an appropriate tuning procedure to maximal twist, lattice artefacts indeed follow the expected $\mathcal{O}(a^2)$ scaling behaviour.

A comprehensive simulation programme has been undertaken by the European Twisted Mass (ETM) collaboration, including dynamical simulations with $N_{\rm f} = 2$ [36–38] and $N_{\rm f} = 2+1+1$ [39] quark flavours.

At maximal twist, the quark mass is given by the twisted mass μ_q and, as in the case of overlap fermions, it renormalizes multiplicatively with a renormalisation factor $Z_\mu = 1/Z_{\rm P}$. In contrast to standard Wilson fermions, an exact lattice Ward identity for maximally twisted mass fermions allows the extraction of the decay constant of the charged pseudoscalar meson from the relation

$$f_\pi^{\rm tm} = \frac{2\mu_q}{(m_\pi^{\rm tm})^2}\,|\langle 0|P|\pi^\pm\rangle_{\rm tm}|\,,$$

which is free from the presence of renormalisation factors.

The twisted mass term in eq.(4) explicitly breaks parity and isospin symmetry, which are however restored in the continuum limit with a rate of $\mathcal{O}(a^2)$ as shown in [7] and numerically confirmed in [36, 40]. The effect of isospin breaking has been observed to affect in a substantial way only the neutral pion mass. Indeed, while the discretization effects in the charged pion are observed to be small, significant $\mathcal{O}(a^2)$ corrections appear when studying the scaling to the continuum limit of the neutral pion [36]. Similar effects have not been observed in other quantities that are in principle sensitive to isospin breaking but not trivially related to the neutral pion mass. These observations are supported by theoretical considerations detailed in [41, 42].

2.3 Matching Procedure

In order to perform the continuum limit extrapolation, the physical situation (e.g. the quark mass and the lattice size) has to be kept fixed when changing the lattice spacing. In practise, this requires a matching procedure at each value of the lattice spacing. One possibility for this matching is to directly match the renormalized quark masses. Another option is to match a hadronic quantity that can be accurately determined with both regularisation and that depends in a significant way on the quark mass. In the light quark sector, the mass of the pseudo Nambu-Goldstone boson is a natural hadronic observable to perform this matching. In this work we follow this procedure, by defining the matching point in the following way:

$$m_\pi^{\rm ov}|_{m_{\rm ov}\equiv m_{\rm ov}^{\rm match}} = m_\pi^{\rm tm}|_{\mu_q=\mu_q^{\rm sea}}\ , \tag{5}$$

where the l.h.s is the mass of a pseudoscalar meson consisting of mass degenerate overlap valence quarks of mass $m_{\rm ov} = m_{\rm ov}^{\rm match}$ (the so called matching quark mass) in a background of $N_{\rm f} = 2$ twisted mass sea quarks with mass $\mu_q = \mu_q^{\rm sea}$. The mass $m_\pi^{\rm tm}$ in the r.h.s corresponds to the pseudoscalar meson made of twisted mass valence and sea quarks of mass $\mu_q = \mu_q^{\rm sea}$.

To illustrate the matching procedure in the valence sector, we perform a continuum limit scaling analysis of overlap and twisted mass fermions in the free theory.

Illustration in the Free Theory

We want to investigate the effects of the matching procedure of the quark mass in the free theory by using as a matching condition the pseudoscalar meson masses of maximally twisted mass fermions and of overlap fermions. The twisted mass is kept fixed to $N\mu_q = 0.5$, where N is the number of lattice sites in the spatial directions.

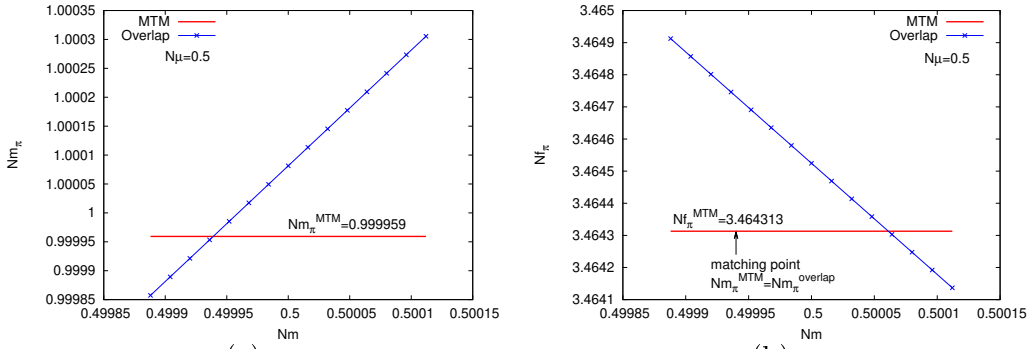


Fig. 1. Tree-level examples : (a) the matching of twisted mass and overlap quark masses and (b) the mismatch between the twisted mass and overlap pseudoscalar decay constants at the matching point $Nm_\pi^{\rm tm} = Nm_\pi^{\rm ov}$.

We illustrate the matching procedure through an example with $N = 16$. In this case, the twisted mass pseudoscalar meson mass is $Nm_\pi^{\rm tm} = 0.999959$. Since the magnitude of $\mathcal{O}(a^2)$ effects is in general different for different fermion discretizations, if we impose the condition of equal pseudoscalar meson masses $Nm_\pi^{\rm tm} = Nm_\pi^{\rm ov}$, the bare quark masses will differ $Nm_{\rm ov} \neq N\mu_q$. This is shown in Fig. 1(a), where the dependence of the overlap pseudoscalar meson mass on the quark mass $Nm_{\rm ov}$ is depicted. The value $Nm_{\rm ov}^{\rm match} \approx 0.49994$ leads to the same pseudoscalar meson mass as the value $N\mu_q = 0.5$ in the twisted mass case.

Since the size of discretization effects depend on the particular observables under consideration, the matching of the pseudoscalar meson mass does not imply that other observables will also be matched. This is illustrated in Fig. 1(b) which shows the difference of the pseudoscalar decay constants at the matching point, $Nm_\pi^{\rm tm} = Nm_\pi^{\rm ov}$.

The difference $Nf_\pi^{\rm tm} - Nf_\pi^{\rm ov}$ vanishes in the continuum limit at a rate of $\mathcal{O}(a^2)$. We consider different lattice sizes, by changing N in the range $N = 4$ to $N = 64$. By fixing the physical situation to $N\mu_q = 0.5$, the change in N introduces the scaling towards the continuum limit, which, in the free theory, corresponds to the limit $N \to \infty$.[3] For each lattice size N, we determine the matching overlap quark mass $Nm_{\rm ov}^{\rm match}$, such that the overlap and twisted mass pseudoscalar meson masses are equal. In Fig. 2 we illustrate the dependence of the difference $Nf_{\rm PS}^{\rm tm} - Nf_{\rm PS}^{\rm ov}$ on $1/N^2$. This difference indeed vanishes in the limit $N \to \infty$ and the leading discretization effects are of $\mathcal{O}(1/N^2)$. A similar behaviour is observed for other observables such as the pseudoscalar correlation function at a fixed physical distance.

[3] More details about tree-level scaling tests of various fermion discretizations and their expressions for the quark propagators and correlation functions can be found in [43, 44].

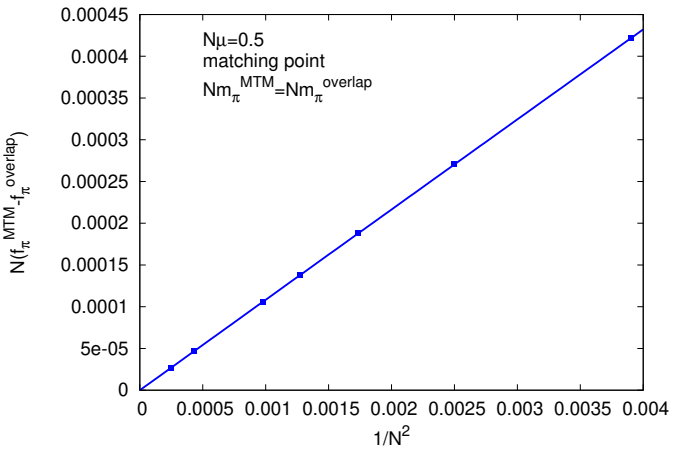


Fig. 2. The difference, in the free theory, between the twisted mass and overlap pseudoscalar meson decay constants at the matching point $Nm_\pi^{\rm tm} = Nm_\pi^{\rm ov}$, as a function of $1/N^2$. The limit $1/N^2 \to 0$ corresponds to the continuum limit.

3 Simulation Setup

In the following, we will investigate the just discussed example of free fermions in the case of including the interaction to the gluon fields. In table 1 we provide the list of dynamical simulations considered in this work. The ensembles were generated by the ETM collaboration [36] using the tree-level Symanzik improved gauge action and $N_{\rm f} = 2$ flavours of maximally twisted mass fermions.

The heavier ensembles labelled in table 1 with a subscript h, i.e. B_h, C_h and D_h, correspond to three values of the lattice spacing with a physical situation fixed to a lattice size $L/r_0 \approx 3$ and a charged pseudoscalar meson mass $m_\pi^{\rm tm} r_0 \approx 1.0$, where r_0 is the Sommer scale [45]. This corresponds to a lattice size $L \approx 1.3\,{\rm fm}$ and a non-perturbatively renormalized [46] quark mass $\mu_q^{\overline{\rm MS}}(\mu = 2\,{\rm GeV}) \approx 40\,{\rm MeV}$. In infinite volume this corresponds to a pseudoscalar meson mass $m_\pi \approx 450\,{\rm MeV}$.

The lighter ensembles are labelled with a subscript ℓ. In this case the pseudoscalar meson mass is fixed to $m_\pi r_0 \approx 0.8$. This corresponds to a quark mass $\mu_q^{\overline{\rm MS}}(\mu = 2\,{\rm GeV}) \approx 20\,{\rm MeV}$, which in infinite volume gives a pseudoscalar meson mass of around 300 MeV. The subscripts $V_{1,2,3}$ refer to ensembles with different spatial lattice extents.

In the valence sector we use overlap fermions [4]. The gauge links entering in the covariant derivative of the kernel operator A in eq. (2) are HYP smeared to reduce the condition number of $A^\dagger A$. The mass parameter s is set to $s = 0$ since this is observed to provide the best locality properties for the overlap

[4] More details about our overlap fermions setup are given in [47].

Ensemble	β	$(L/a)^3 \times T/a$	$a\mu_q$	$\kappa_{\rm crit}$	$m_\pi^{\rm tm} r_0$	L/r_0
B_h	3.90	$16^3 \times 32$	0.0074	0.160856	1.03	3.0
B_{ℓ,V_1}		$16^3 \times 32$	0.0040		0.84	
B_{ℓ,V_2}		$20^3 \times 40$			0.73	3.8
B_{ℓ,V_3}		$24^3 \times 48$			0.72	4.6
C_h	4.05	$20^3 \times 48$	0.0060	0.157010	1.00	3.0
C_ℓ		$20^3 \times 40$	0.0030		0.83	
D_h	4.20	$24^3 \times 48$	0.0050	0.154073	1.04	2.9
D_ℓ		$24^3 \times 48$	0.0020		0.82	

Table 1
Summary of $N_{\rm f} = 2$ Wilson twisted mass ensembles considered in this work. We give the ensemble label, the values of the inverse coupling β, the lattice volume $L^3 \times T$, the twisted mass parameter $a\mu_q$, the critical hopping parameter $\kappa_{\rm crit} = 1/(8 + 2am_{\rm crit})$, the approximate values of the pseudoscalar meson mass and of the lattice size in units of the Sommer scale r_0. The chirally extrapolated values of the Sommer scale are $r_0/a = 5.25(2)$ at $\beta = 3.90$, $r_0/a = 6.61(2)$ at $\beta = 4.05$ and $r_0/a = 8.33(5)$ at $\beta = 4.20$, corresponding to lattice spacings $a \approx 0.079\,$fm, $a \approx 0.063\,$fm and $a \approx 0.051\,$fm, respectively [36]. The subscripts h and ℓ in the ensemble name refer to the heavy and light quark masses, respectively, which are kept fixed when performing the continuum limit extrapolation. The subscripts $V_{1,2,3}$ label ensembles with different lattice sizes.

operator [5].

For each dynamical quark ensemble in table 1, we produce all-to-all overlap quark propagators in a wide range of quark masses $m_{\rm ov}$, from the unitary (sea) light quark mass up to the physical strange quark mass. This provides a good handle on the matching procedure, to be discussed in the following section. Note that the lattice size $L/r_0 \approx 3$ is outside the regime of applicability of chiral perturbation theory (or its generalisation to mixed actions). In this work, we instead rely on a direct study of the continuum limit of the mixed action in order to characterise the size of unitarity violations.

[5] Preliminary results were presented in [48] and we refer to a forthcoming publication [49] for more details about this aspect.

4 Continuum Limit Scaling Tests and Different Matching Conditions

In this section, we will discuss a number of continuum limit scaling tests for the pseudoscalar decay constant. We will employ three different matching conditions to relate the overlap valence quarks to the maximally twisted mass sea quarks and the pseudoscalar decay constant will be extracted from two different correlation functions which differ by their sensitivity to chiral zero modes. We remark that we consider the matching condition employed *to define* the mixed action theory used. This is similar to improvement conditions where the resulting improvement coefficients define the improved actions and operators. In particular, there is then no uncertainty associated with a given matching condition. However, it is of course still important to investigate different matching conditions and study their effects, as we will do in this work.

In the following we will use the shorthand notation "scaling test" for the continuum limit scaling test in the lattice spacing. As in the example of free fermions discussed above, we start with a *naive scaling test*. Demonstrating that such naive procedure leads to a problem, when the continuum limit is taken, we will introduce an *improved scaling test*. By also discussing an *alternative scaling test*, we will then demonstrate that physical results and the approach to the continuum limit can strongly depend on the choice of the setup for a scaling test. We provide an explanation for this finding by the effects of exact chiral zero modes of the overlap Dirac operator taken in the valence sector.

4.1 Naive Scaling Test

The *naive scaling test* follows very closely the example of free fermions discussed above. As in the free case, we match the pseudoscalar meson masses computed from the correlator constructed from the pseudoscalar interpolating field (PP correlator, $C_{\rm PP}(t)$), which appears to be the most natural choice. Of course, in practical simulations, the pseudoscalar masses cannot not be matched exactly. We therefore use that value of the overlap pseudoscalar mass which is closest to the targeted twisted mass value. The corresponding overlap bare quark mass then defines our matching quark mass. Using $C_{\rm PP}(t)$ for the matching condition we will refer to as *naive matching condition*. To proceed, we evaluate the pseudoscalar correlation function $C_{\rm PP}(t)$ for light quark masses using ensembles B_{ℓ,V_1}, C_ℓ and D_ℓ.

The matching procedure is illustrated for the case B_{ℓ,V_1} in Fig. 3(a). The values of the matching quark and pseudoscalar masses obtained from different

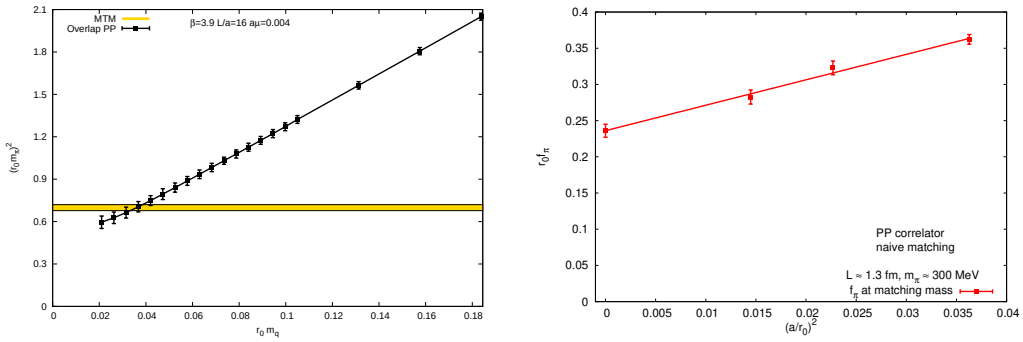
Ensemble ↓ matching →	am_π	$am_{\rm ov}^{\rm match}$ naive	$am_{\rm ov}^{\rm match}$ improved	$am_{\rm ov}^{\rm match}$ alternative
B_h	0.1961(17)	0.015	0.016	0.017
B_{ℓ,V_1}	0.1592(24)	0.007	0.011	0.009
B_{ℓ,V_2}	0.1389(14)	0.007	0.009	—
B_{ℓ,V_3}	0.1359(7)	0.008	0.008	—
C_h	0.1520(15)	0.011	0.012	0.013
C_ℓ	0.1209(40)	0.005	0.006	0.006
D_h	0.1252(13)	0.009	0.010	0.010
D_ℓ	0.0980(19)	0.002	0.004	0.004

Table 2
The pseudoscalar masses and overlap matching quark masses for different ensembles. Results of employing different matching conditions are shown.

ensembles are tabulated in table 2. In Fig. 3(b) we show the pseudoscalar decay constant computed from the valence overlap fermions at the matching mass as a function of a^2. As in the case of free fermions, we indeed find a scaling of the pseudoscalar decay constant compatible with the expected $O(a^2)$ behaviour. However, we encounter a problem with this naive scaling test when extrapolating the mixed action pseudoscalar decay constants to the continuum limit, we find $r_0 f_\pi^{\rm ov} = 0.236(9)$ while the continuum extrapolated value for unitary twisted mass fermions comes out to be $r_0 f_\pi^{\rm tm} = 0.181(10)$.

Thus, it seems that we are obtaining an inconsistent continuum limit from our mixed action simulation. Of course, this observation demands an explanation, since this is clearly in contradiction to our expectation and must be an artifact of our setup. Indeed, the setup of our naive scaling test is too naive. It does not take into account the above mentioned mismatch of the eigenvalue spectra of the lattice Dirac operators. In particular, the pseudoscalar correlator might be strongly affected by zero modes of the overlap Dirac operator, especially in the small volume and at the small value of the quark mass employed by using ensembles B_{ℓ,V_1}, C_ℓ and D_ℓ.

The suspicion of the overlap zero modes being responsible for the apparent inconsistent continuum limit values for the pseudoscalar decay constant leads to an *improved scaling test*.



(a) (b)

Fig. 3. (a) Naive matching condition for the case of ensemble B_{ℓ,V_1}. (b) Continuum limit of f_π in the case of the naive matching condition.

4.2 Improved Scaling Test

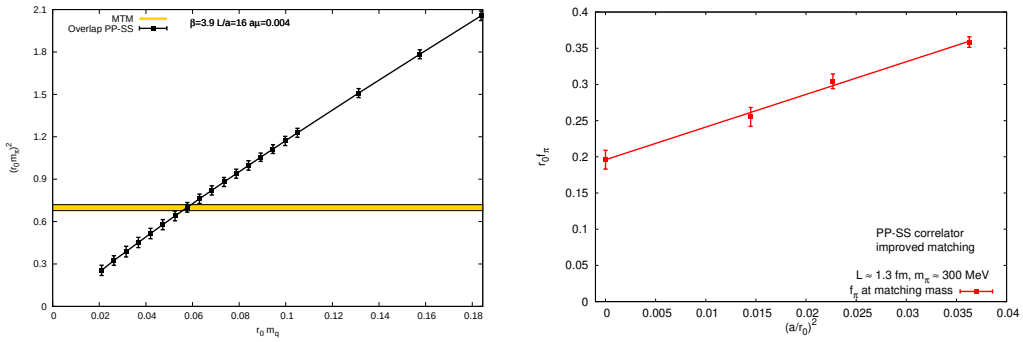
In order to check the assumption that the zero modes play a special rôle in our mixed action setup, we should use observables for which such zero mode contributions are cancelled and which are therefore in this sense "improved". Such observables can then be used both in the matching condition and to compute the physical quantity. As we will demonstrate below, once an improved version of –in our case– f_π is used, all matching conditions considered lead to completely consistent continuum limit values.

Our improved scaling test consists of studying instead of the pure pseudoscalar correlation function the correlator

$$C_{\mathrm{PP-SS}}(t) \equiv C_{\mathrm{PP}}(t) - C_{\mathrm{SS}}(t)\,, \tag{6}$$

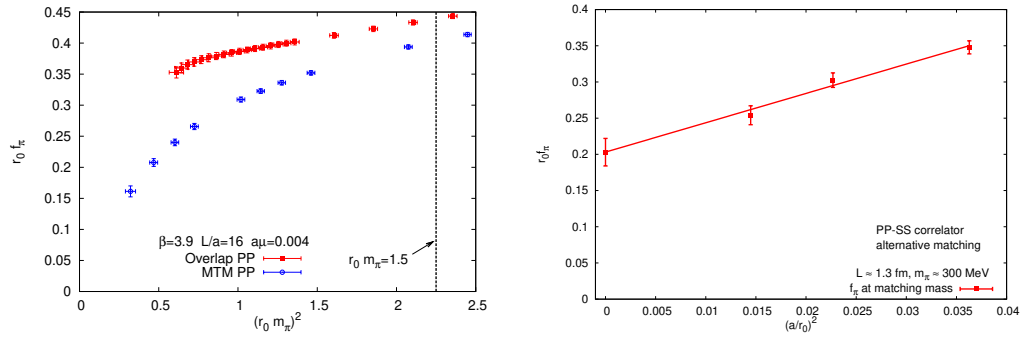
where the scalar correlation function is subtracted and hence the contribution of zero modes is exactly cancelled, since they are eigenfunctions of γ_5. In this way, we match the overlap (mixed action) pseudoscalar meson mass resulting from such correlator to a unitary pseudoscalar meson mass extracted from the standard PP correlator. This defines the *improved matching condition*. Moreover, we extract f_π^{ov} from the PP-SS correlator. Therefore, we have an improved setup in both the matching condition and in the observable itself – in both we avoid the effects of zero modes.

We show the matching of the pseudoscalar mass in Fig. 4(a) and the scaling in a^2 of the pseudoscalar decay constant in Fig. 4(b) where we again observe the expected $\mathcal{O}(a^2)$ scaling behaviour. Performing a continuum limit extrapolation of f_π, we find $r_0 f_\pi^{\mathrm{ov}} = 0.196(13)$ which is now completely compatible with the one of twisted mass fermions, $r_0 f_\pi^{\mathrm{tm}} = 0.181(10)$.



(a) (b)

Fig. 4. (a) Improved matching condition for the case of ensemble B_{ℓ,V_1}. (b) Continuum limit of f_π in the case of the improved matching condition.



(a) (b)

Fig. 5. (a) Matching of overlap and MTM quark masses (ensemble B_{ℓ,V_1}) at a heavy quark mass value (yielding $r_0 m_\pi = 1.5$, which is denoted by vertical line), where the zero modes effects are strongly suppressed. Idea of the matching is explained in the text. (b) Continuum limit of f_π in the case of the alternative matching condition.

4.3 Alternative Scaling Test

The results of the previous two sections indicate that indeed the zero modes play a special rôle in the mixed action setup used here. Using the correlator $C_{\mathrm{PP-SS}}(t)$ which cancels the zero mode contributions exactly is not the only possibility to reach this goal. Our alternative scaling test starts by the observation that zero modes can also be suppressed by using either a large enough volume or large quark masses, see also the discussion below. One way of avoiding the effects of chiral zero modes, at least in the matching condition, is then to match the theories at a heavy quark mass values where the effect of the zero modes is strongly suppressed.

An idea of such matching is the following. We choose a value of $r_0 m_\pi = 1.5$ in the regime of quark masses where the difference between the $C_{\mathrm{PP}}(t)$ and $C_{\mathrm{PP-SS}}(t)$ correlators is negligible, which indicates that the effects of the zero modes are small. The dependence of the pseudoscalar mass on the overlap

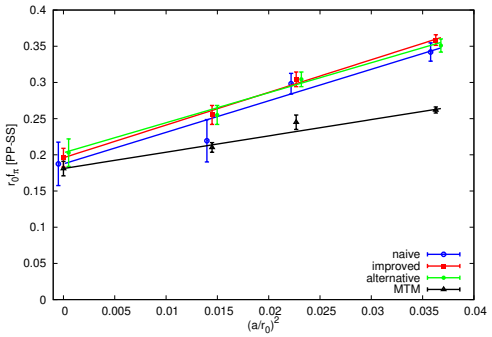


Fig. 6. Continuum limit scaling of $r_0 f_\pi$, using different matching conditions and extracting f_π from the PP-SS correlator. All matching conditions lead to a consistent continuum limit with the one of the unitary approach. In the graph the data for "naive matching" is shifted to the left and the data for "alternative matching" to the right, for reasons of a better presentation.

and MTM quark mass (using partially quenched MTM data) allows us to find the values of quark masses which correspond to the chosen value of $r_0 m_\pi$. As can be seen on Fig. 5(a), the smallness of the zero modes effects at this value of $r_0 m_\pi$ means that the difference $r_0(f_\pi^{\rm ov} - f_\pi^{\rm tm})$ is significantly reduced with respect to the large difference in $r_0 f_\pi$ in the small quark mass regime. The ratio of MTM and overlap bare quark masses that lead to $r_0 m_\pi = 1.5$ provides an estimate of the ratio $R_{Z_P} \equiv Z_{\rm P}^{\rm ov}/Z_{\rm P}^{\rm tm}$. In this way, we can define the *alternative* matching mass as $R_{Z_P}\mu_q$, where μ_q is the unitary MTM quark mass. The values that we find from this procedure (for all ensembles with linear lattice extent $L \approx 1.3$ fm) are again tabulated in table 2.

Once we have the matching masses from the alternative matching condition, we can perform the continuum limit scaling of the corresponding decay constant, extracted again from the $C_{\rm PP-SS}(t)$ correlator, such that the zero modes effects are suppressed both in the matching condition and in the values of f_π (in this sense, such setup is again an improved one with respect to the naive scaling test). Needless to say that we again observe a nice $O(a^2)$ scaling of the pseudoscalar decay constant towards the continuum limit (Fig. 5(b)), where we find $r_0 f_\pi^{\rm ov} = 0.203(19)$, which is to be compared to the continuum limit value of twisted mass fermions $r_0 f_\pi^{\rm tm} = 0.181(10)$. Again, a consistent result is found. Note that a similar conclusion is obtained if instead of performing the alternative matching with partially quenched data, we use the unitary ensembles B_h, C_h and D_h, at the heavier masses, to impose the matching condition.

5 Interpretation and Discussion

In the previous section, we have discussed continuum limit scaling tests, employing three different matching conditions and using two definitions for $f_\pi^{\rm ov}$. The disturbing observation in these scaling tests has been that in case of the naive scaling test, an apparent inconsistency of the continuum limit value of f_π has been encountered which, however, could be resolved by employing an improved and an alternative scaling strategy. One may wonder then, whether in the naive scaling test the matching condition, the used observable or even some interplay between both are responsible for the inconsistent continuum limit of f_π.

Fig. 6 provides an answer to this question, at least in the case of f_π considered here. In the graph, we use the naive, improved and alternative matching conditions but evaluate $f_\pi^{\rm ov}$, in all cases, from $C_{\rm PP-SS}(t)$. Obviously, with all three matching conditions we obtain a completely consistent continuum limit value of $f_\pi^{\rm ov}$, agreeing well with the one from the unitary setup. Thus, it seems that the choice of the observable has a significant impact on the observed mismatch in the naive scaling test of f_π due to the zero modes effects.

It is interesting to also perform the opposite test by using again all three matching conditions but this time only use $f_\pi^{\rm ov}$ computed from the PP correlator. In this case, we obtain inconsistent continuum limit values, $r_0 f_\pi^{\rm ov} = 0.236(9)$, $r_0 f_\pi^{\rm ov} = 0.252(10)$ and $r_0 f_\pi^{\rm ov} = 0.256(10)$ for the naive, improved and alternative matching conditions, respectively, while for the unitary setup we have the value $r_0 f_\pi^{\rm tm} = 0.181(10)$. As a consequence, it is important to define observables such that they are not influenced by zero modes.

As we have shown above, mixed actions involving chiral fermions only in the valence sector can exhibit particular effects. Indeed, the spectra of overlap and twisted mass Dirac operators differ in an essential way. The overlap Dirac operator, being chirally symmetric, incorporates the physical effects of exact chiral zero modes at any value of the lattice spacing. This is not the case for the Wilson twisted mass Dirac operator. In the context of a mixed action this implies that the effect of zero modes in the valence sector is not properly suppressed by a fermionic determinant which depends only on sea quarks. Zero mode effects can therefore introduce potential difficulties when comparing the continuum limit extrapolation of mixed action data with respect to the unitary case.

The effects of zero modes are observable dependent. In particular, when aiming at studies of QCD on a large volume, an appropriate choice of the interpolating operator can be used to reduce or to cancel the effects of zero modes on a given observable. Indeed, zero modes effects can be interpreted as finite size

effects and are thus suppressed as the volume is increased. Moreover, when the quark mass increases, the relative contribution of the zero modes decreases with respect to the one of the other low-lying modes. Observables receiving contributions from zero modes are therefore less influenced by their effects as the quark mass increases.

Before closing this section, we collect a few remarks about the continuum limit scaling of the mixed and unitary actions.

- The previous sections and discussion have illustrated the influence of exact zero modes of the overlap operator in a mixed action setup. We have examined three examples of continuum limit scalings which give partially different results. Of course, our list is by no means exhaustive, nor do we claim to have provided the "optimal" continuum limit strategy. However, we have clearly provided a warning that in a mixed action setup special care has to be taken when lattice Dirac operators with exact chiral zero modes are employed in the valence sector. In the following, we will make an attempt to provide a quantitative estimate in the region of volume and pseudoscalar mass where the zero modes are the dominant effect and where they can be safely neglected.
- The $C_{\mathrm{PP-SS}}(t)$ correlator in eq. (6) has different discretization effects than $C_{\mathrm{PP}}(t)$. Indeed, it is known that the scalar correlator $C_{\mathrm{SS}}(t)$ is especially vulnerable to the double pole contribution to the meson propagator [22]. This unphysical effect is present in all unitarity violating setups (quenched, partially quenched and mixed action) and a separate analysis indicates that the scalar correlator indeed obtains a negative contribution of this kind, which has opposite sign with respect to the one from zero modes [49].
- The $C_{\mathrm{PP-SS}}(t)$ correlator receives excited state contributions from the scalar correlator. This can affect the extraction of the pseudoscalar ground state in the large quark mass region. In the regime of quark masses that we consider in this work this appears to be a negligible effect. In general, we observe clear signals for the plateaux, which we have furthermore controlled by comparing the extracted values of m_π and f_π to an analysis including an estimate of the systematic effect due to the choice of the fit interval, see also [49].
- For twisted mass fermions, the use of $C_{\mathrm{PP-SS}}(t)$, instead of $C_{\mathrm{PP}}(t)$, has a negligible impact on the values of f_π and m_π in the regime of parameters (quark mass, lattice size and lattice spacing) that we consider in this work. We only consider the latter case.
- In the Wilson twisted mass formulation, a potential contribution from the large discretization effects present in the neutral pion mass can occur, in particular through finite volume effects. However, these cut-off effects are in principle properly taken into account by the fact that both the quark mass and the volume are kept fixed during the continuum limit extrapolation. The fact that we observe the expected $\mathcal{O}(a^2)$ scaling behaviour, gives us

Ensemble	$r_0 f_\pi$ unitary MTM PP correlator	$r_0 f_\pi$ naive matching PP correlator	$r_0 f_\pi$ improved matching PP-SS correlator
B_h	0.3413(33)	0.3973(65)	0.3626(107)
C_h	0.3373(33)	0.3774(63)	0.3669(78)
D_h	0.3382(50)	0.3493(100)	0.3558(90)
continuum limit	0.334(11)	0.330(17)	0.345(18)

Table 3
The values of the pseudoscalar decay constant for ensembles B_h, C_h and D_h at the matching mass (with the naive and improved matching condition). The continuum limit values are also shown.

confidence that potential isospin breaking effects are indeed removed in the continuum limit, as also observed in [36].

6 Quark Mass Dependence and Finite Size Effects

In this section, we will perform a matching of the twisted mass sea and valence overlap actions at a heavier quark mass and at larger volumes. The purpose of this investigation is twofold. First of all, these investigations will tell us on a quantitative level at which value of the quark mass and volume the effects of the exact chiral zero modes are harmless (safe region), when their effect is significant (hazardous region) and when their effect is unacceptably large (non-safe region). Second, using larger quark masses and volumes serves as a test of the picture developed in the previous sections about the rôle of the zero modes in a mixed action simulation.

6.1 Quark Mass Dependence

For the matching of the heavier quark mass we use the ensembles B_h, C_h and D_h of table 1. We apply for these ensembles both the naive matching procedure (naive matching condition using f_π from the PP correlator) and the improved one (improved matching condition using f_π from the PP-SS correlator). In both cases we observe, as expected, a nice scaling of the pseudoscalar decay constant in a^2 towards the continuum limit. In table 3 we give the values of the pseudoscalar decay constants from the naive and the improved matching conditions, as well as one for the unitary twisted mass case. As can be seen in

the table, the differences in the values of $f_\pi^{\rm ov}$ and $f_\pi^{\rm tm}$ for all ensembles are much smaller than in the case of B_{l,V_1}, C_l and D_l ensembles and all continuum limit values are consistent with one another. This clearly confirms our interpretation that the zero modes effects are large at a quark mass corresponding to a pseudoscalar mass of 300 MeV (in infinite volume). At 450 MeV, these effects are strongly suppressed although not totally negligible (see table 3).

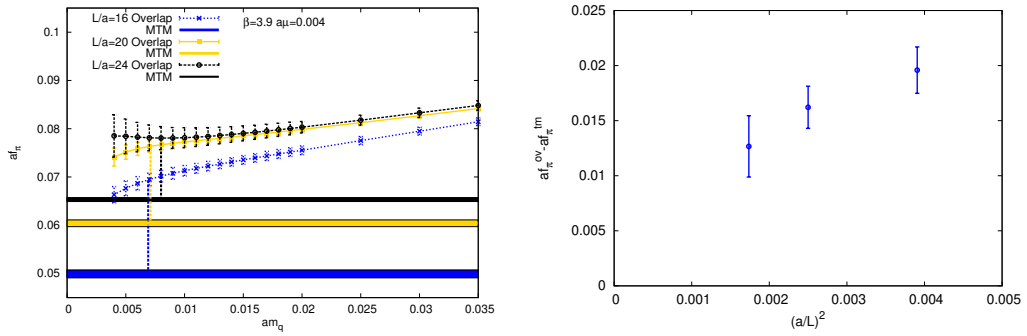
6.2 Finite Size Effects

Finite size effects (FSE) in the light pseudoscalar meson observables considered in this work can have multiple origins. As mentioned earlier, zero modes of the Dirac operator can introduce significant finite volume effects in the pseudoscalar correlator. Other sources of FSE are related to pion loops or to the actual size of the box with respect to the typical hadronic scale. Concerning pion loops, in the case of twisted mass fermions a contribution to FSE from the lighter neutral pion mass can in principle be present at finite lattice spacing, although this is expected to vanish when performing the continuum limit extrapolation (as discussed in the previous section). When considering the scalar correlator, an additional FSE arises from the bubble diagram describing the exchange of two pseudoscalar mesons. Isolating the relative contribution of these effects in our data for the mixed and unitary actions is beyond the scope of this work. Here, we rather concentrate on the comparison of the dependence of $f_\pi^{\rm tm}$ and $f_\pi^{\rm ov}$ on the volume, since this should give some evidences of the presence of FSE from the topological zero modes.

We consider three ensembles B_{ℓ,V_1}, B_{ℓ,V_2}, B_{ℓ,V_3} at the coarsest value of the lattice spacing, see table 1. The corresponding linear lattice extents are 1.3 fm, 1.7 fm and 2.0 fm, respectively. The quark mass is set to $m_q \approx 20\,\mathrm{MeV}$ and the values of $m_\pi L$ at the matching point are 2.5, 2.8, 3.3, for ensembles B_{ℓ,V_1}, B_{ℓ,V_2}, B_{ℓ,V_3}, respectively.

To illustrate the magnitude of finite size effects, we plot the quark mass dependence of the pseudoscalar meson decay constant – in this section we only use the PP correlator – for our three ensembles in Fig. 7(a). The horizontal bands correspond to the unitary values of $f_\pi^{\rm tm}$. The matching mass (employing the naive matching procedure) is shown by the vertical dashed line. We observe significant FSE for both the mixed and unitary actions when reducing the lattice size from 1.7 fm down to 1.3 fm, while they are smaller between 2.0 fm and 1.7 fm. Note that for f_π there is a relative sign in the contribution to FSE coming from pion loops and zero modes. This could induce, in practise, some cancellations of FSE in the mixed action data.

The differences between the decay constants $f_\pi^{\rm ov}$ and $f_\pi^{\rm tm}$, at the matching



(a) (b)

Fig. 7. Finite size effects from ensembles B_{ℓ,V_1}, B_{ℓ,V_2}, B_{ℓ,V_3} (see table 1). (a) Quark mass dependence of the pseudoscalar meson decay constant. (b) Volume dependence of the difference between the pseudoscalar meson decay constant in the mixed and unitary actions. We observe that the difference between $f_\pi^{\rm tm}$ and $f_\pi^{\rm ov}$ decreases when increasing the volume.

mass, are plotted in Fig. 7(b). In such difference, many of the contributions to FSE are expected to cancel. The fact that $f_\pi^{\rm ov} - f_\pi^{\rm tm}$ has a non vanishing slope when changing the lattice size can be interpreted as a FSE coming from the zero modes of the overlap operator. This hypothesis is supported by the fact that this slope is within errors compatible with zero when instead of using $f_\pi^{\rm ov}[\mathrm{PP}]$ in the difference, one considers $f_\pi^{\rm ov}[\mathrm{PP}-\mathrm{SS}]$, extracted from the $C_{\mathrm{PP}-\mathrm{SS}}(t)$ correlator.

Fig. 7(b) provides indications that FSE from topological zero modes are not totally negligible for the ensemble B_{ℓ,V_3}, with our largest lattice size $L \approx 2.0\,\mathrm{fm}$ and $m_\pi L \approx 3.3$. For the heavier ensemble B_h, with $L \approx 1.3\,\mathrm{fm}$ and $m_\pi L \approx 3.1$ and the same value of the lattice spacing, we observed that $af_\pi^{\rm ov} - af_\pi^{\rm tm} = 0.011(1)$, arising mainly from unitarity violations, since zero mode effects were observed to be small in this case. By taking this value as a rough estimate for the size of unitarity violations at this value of the lattice spacing, we estimate that a lattice size $L \geq 2.4\,\mathrm{fm}$ (corresponding to $m_\pi L \geq 4$) would be needed, at the lighter quark mass $m_q \approx 20\,\mathrm{MeV}$, to enter in the regime of small FSE from chiral zero modes. In practise, this would require to deal with the overlap operator on an $L/a = 32$ lattice.

We close this section by a remark about the size of the unitarity violations in our mixed action. The difference $f_\pi^{\rm ov} - f_\pi^{\rm tm}$ in Fig. 7(b) is numerically large for all three volumes. This difference is not expected to vanish in the infinite volume limit due to the presence of unitarity violations in the mixed action data at non-zero values of the lattice spacing. At a value of the lattice spacing, $a \approx 0.08\,\mathrm{fm}$, with $L \approx 2.0\,\mathrm{fm}$ and $m_\pi L \approx 3.3$, we observe that the mixed and unitary values of f_π can differ by 20%. Fig. 6 illustrates a similar effect on a smaller volume. Indeed a significant difference between overlap and twisted-mass data is observed at the coarser value of the lattice spacing, $a \approx 0.08\,\mathrm{fm}$.

This points towards the necessity of a proper control of the continuum limit extrapolation when working in a mixed action setup.

7 Conclusion

We have studied the continuum limit scaling of a mixed action with overlap valence quarks on a twisted mass sea employing three values of the lattice spacing. We observe the expected $O(a^2)$ scaling behaviour for the here investigated pseudoscalar decay constant. We have demonstrated that in such mixed action approach the zero modes of the overlap operator which are unmatched by the twisted mass operator at the lattice spacings employed here, can play a special rôle. They can severely affect physical quantities such as the pseudoscalar decay constant.

The precise values of the quark mass and/or lattice size at which the effects of zero modes become relevant for a given observable are not known a priori. A dedicated numerical study is therefore needed to address this question. To this end, we performed simulations at two values of the quark mass and three volumes. These calculations then provided information on the values of the parameters for which these zero mode effects are significant or when they can be neglected. Our findings are summarised in Fig. 8. There we indicate on a more qualitative level the regions in the quark mass and volume where simulations ought to be safe, i.e. where the zero modes play no significant rôle, the hazardous regions, where their effect can be significant and a non-safe region, where their effect become really large.

We want to stress that the difficulties in the continuum limit approach of f_π arising from the zero modes of the overlap Dirac operator originate solely from the particular definition of f_π and not from the matching condition employed. We demonstrated this clearly by, employing three different matching conditions, but using only a definition of $f_\pi^{\rm ov}$ (constructed from $C_{\rm PP-SS}(t)$) which is not affected by zero modes, see Fig. 6. On the contrary, by employing a definition of $f_\pi^{\rm ov}$ which is highly sensitive to zero modes (i.e. constructed from $C_{\rm PP}(t)$), we find inconsistent continuum limit results for all three matching conditions employed. This might suggest that if it is possible to construct physical observables such that they are not affected by zero modes consistent continuum limit values can be obtained. However, this expectation needs further corroboration by studying other physical quantities.

The effects of zero modes depend on the choice of the operator. Furthermore, their effects vary from one observable to another. We refer to a forthcoming publication [49] for a study of the impact of zero modes on other observables and operators. For some observables, isolating the contribution from

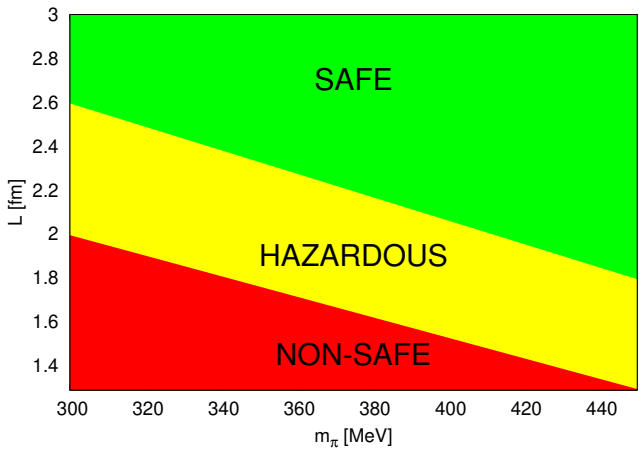


Fig. 8. A qualitative graph indicating the safe, hazardous and non-safe regions of parameters in physical units (linear extent of the lattice vs. pseudoscalar meson mass) in mixed action simulations with overlap valence and twisted mass sea quarks. The parameter values in the "safe" region are such that the effects of chiral zero modes of the overlap operator are negligible. The boundary between the "safe" and "hazardous" region corresponds to $m_\pi L = 4$ and the boundary between "hazardous" and "non-safe" is $m_\pi L = 3$.

zero modes can be a difficult task. For the study of such observables, it is particularly important to perform the simulations in a regime of parameters where these effects are negligible.

By working in the safe regime, where the effects of zero modes are negligible, we believe that this mixed action approach should allow to obtain accurate determinations of quantities for which good chiral properties of valence fermions are essential, such as the kaon bag parameter B_K or the amplitudes of $K \to \pi\pi$ decays.

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