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Scaling test for Wilson twisted mass QCD

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Abstract

We present a first scaling test of twisted mass QCD with pure Wilson quarks for a twisting angle of $\pi/2$. We have computed the vector meson mass $m_{\rm V}$ and the pseudoscalar decay constant $F_{\rm PS}$ for different values of β at fixed value of $r_0 m_{\rm PS}$. The results obtained in the quenched approximation are compared with data for pure Wilson and non-perturbatively O(a) improved Wilson computations. We show that our results from Wilson twisted mass QCD show clearly reduced lattice spacing errors, consistent with O(a) improvement and without the need of any improvement terms added. These results thus provide numerical evidence of the prediction in ref. [1].

1 Introduction

Formulating QCD on a space-time lattice admits a substantial amount of freedom in discretising the continuous derivative with restrictions coming from obeying principles such as gauge invariance, locality and unitarity. Naturally, as long as universality holds, all these formulations should provide consistent results in the limit when the discretisation is removed. The standard Wilson formulation of lattice QCD [2] is a simple realisation of such a discretised version of QCD and has been used for a long time in lattice simulations. However, it has been realised that this formulation has a number of severe problems: it shows large discretisation effects [3] that are linear in the lattice spacing a, it violates chiral symmetry strongly and develops unphysical small eigenvalues of the corresponding lattice Wilson-Dirac operator, even at rather large values of the quark mass.

The problem of discretisation effects can be overcome following the Symanzik improvement program [4, 5], introducing the well known clover term [6] to get full, on-shell $\mathrm{O}(a)$ improved results, if the improvement is performed non-perturbatively [3]. In this approach then also the chiral properties are improved, although chiral symmetry breaking and $\mathrm{O}(a^2)$ lattice spacing effects are still left in the theory and have to be extrapolated away. Despite the fact that non-perturbatively improved Wilson fermions clearly diminish discretisation errors, they, unfortunately, show the same – if not worse – problem of the appearance of small eigenvalues of the lattice Dirac operator [7].

In order to solve the problem of small eigenvalues, it has been proposed in [8] to use the so-called twisted mass formulation of QCD. In this approach the mass term in the Dirac operator is chirally twisted [8], see also [9]. When using such a chirally twisted lattice action in combination with the clover term and a non-perturbatively tuned value of the improvement coefficient, the theory is $\mathrm{O}(a)$ improved and the corresponding lattice Dirac operator is safe against developing small eigenvalues.

Recently, it has been realised [1] that all the above properties of non-perturbatively improved, twisted mass QCD can also be obtained *when the clover term is completely omitted.* If a special value of the twisting angle is chosen one theoretically obtains $\mathrm{O}(a)$ improved results *without adding improvement terms.* At the same time, the lattice Dirac operator is still protected against the appearance of small eigenvalues by construction. This curious observation receives a special importance for simulations with dynamical quarks: In [10] it was found that dynamical fermion simulations with non-perturbatively improved Wilson fermions show signs of first order

phase transitions which render simulations very difficult and induce large cut-off effects.

Although by varying the form of the gauge actions [11] the first order phase transition seems to vanish, it is unclear, whether eventually such phenomena will reappear. The problem of the presence of the first order phase transition may be related to the fact that the clover term in the fermion action generates an adjoint gauge action. Therefore, if $\mathrm{O}(a)$ improvement can be achieved without the clover term, as anticipated in [1], the problems connected to such phase transitions should be completely eliminated. As a consequence, the potential of twisted mass fermions in general may be very large. Since the small eigenvalues are regulated by the twisted mass parameter, simulations at much lower quark masses than used today could be performed with promising, but hard to estimate, advantages to explore the chiral limit of lattice QCD.

In this paper we provide a first test of the conjecture of $\mathrm{O}(a)$ improvement of Wilson twisted mass QCD in quenched numerical simulations. For this purpose we performed a scaling test of the vector meson mass m_{V} and the pseudoscalar decay constant F_{PS} at a fixed value of the physical pseudoscalar mass m_{PS}. We compare the results with those that have been obtained for standard Wilson fermions, see [12] and references therein, and non-perturbatively improved clover fermions [13].

2 Twisted mass QCD with Wilson quarks

In twisted mass QCD (tmQCD) as formulated in [8] the twisted mass action in the continuum reads as follows:

$$S_F[\psi,\bar{\psi}] = \int d^4x \bar{\psi}(D_\mu\gamma_\mu + m_0 + i\mu_q\gamma_5\tau^3)\psi \ , \tag{2-1}$$

where D_μ denotes the usual covariant derivative, m_0 is the standard bare quark mass, τ^3 is the third Pauli matrix acting in flavour space and μ_q is the twisted mass parameter, also referred to as the *twisted mass*.

An axial transformation,

$$\psi' = \exp(i\omega\gamma_5\tau^3/2)\psi, \qquad \bar{\psi}' = \bar{\psi}\exp(i\omega\gamma_5\tau^3/2) \ , \tag{2-2}$$

with a real rotation angle ω leaves the form of the action invariant and merely changes the mass parameters into m_0' and μ_q',

$$\begin{aligned} m_0' &= m_0\cos(\omega) + \mu_q\sin(\omega) \\ \mu_q' &= -m_0\sin(\omega) + \mu_q\cos(\omega) \ . \end{aligned} \tag{2-3}$$

The standard action ($\mu_q' = 0$) is obtained by setting $\tan\omega = \mu_q/m_0$. Note that τ^3 is traceless and therefore the transformation (2-2) does not couple to the fermion determinant anomaly.

In order to have an O(a) improved twisted mass lattice action, it appears to be natural to discretise the Dirac operator adding appropriate improvement terms to the standard Wilson-Dirac operator. Indeed, it has been shown in [14, 15, 16, 17] that by adding the usual clover term, full on-shell O(a) improvement can be obtained.

In [1] it has been realised later that using simply the standard lattice Dirac operator D_W one can obtain O(a) improved physical observables without adding improvement terms. More precisely, it is possible to obtain O(a) improved lattice results by employing only the standard massless Wilson-Dirac operator,

$$D_W = \frac{1}{2}\{\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - ar\nabla^*_\mu\nabla_\mu\} \tag{2-4}$$

under the condition that one averages over physical observables that are obtained from simulations at positive and negative values of the Wilson parameter r. A less general, but similar suggestion was made by the authors of refs. [18, 19]. Instead of using positive and negative values of r, quark masses with different signs may be used: the bare quark mass m_0 can be written as

$$m_0 = m_c(r) + m_q \ , \qquad \text{with} \qquad m_c(-r) = -m_c(r) \ , \tag{2-5}$$

where $m_c(r)$ is the critical quark mass, and m_q is the subtracted bare quark mass. Averaging physical observables obtained from simulations at positive and negative subtracted bare quark masses, again O(a)-improvement is obtained.

Let us shortly sketch the arguments leading to this surprising result. One first has to observe that with

$$\mathcal{R}_5 : \begin{cases} \psi & \to \ \psi' = \gamma_5\psi \\ \bar\psi & \to \ \bar\psi' = -\bar\psi\gamma_5 \end{cases} \tag{2-6}$$

the following combined transformation

$$\mathcal{R}_5^{\mathbf{sp}} \equiv \mathcal{R}_5 \times [r \to -r] \times [m_q \to -m_q] \tag{2-7}$$

is a so called *spurionic* symmetry of the ordinary Wilson action. Another symmetry of the Wilson (and Wilson tmQCD) action is $\mathcal{R}_5 \times \mathcal{D}_d$. In the continuum, the transformation $\mathcal{D}_d$ has the effect of changing the sign of all the

space-time coordinates and multiplies each local term $\mathcal{L}_i$ in the Lagrangian density by the factor $(-1)^{d[\mathcal{L}_i]}$, where $d[\mathcal{L}_i]$ is the naive dimension of $\mathcal{L}_i$. The lattice version of this transformation is more involved and we refer to ref. [1] for details.

Taking now the parity properties of multiplicatively renormalisable operators under $\mathcal{R}_5^{\mathbf{sp}}$ and $\mathcal{R}_5 \times \mathcal{D}_d$ into account, one can show – using the Symanzik expansion – that one gets $\mathrm{O}(a)$ improvement when averaging over two simulations with positive and negative Wilson coefficient r (Wilson average (WA)). In addition, from the spurionic symmetry $\mathcal{R}_5^{\mathbf{sp}}$ of the Wilson (and Wilson tm) action one can obtain $\mathrm{O}(a)$ improved physical observables when averaging, at a fixed value of r, over two simulations with positive and negative m_q, as defined in eq. (2-5) (mass average (MA)), taking into account this time the $\mathcal{R}_5$-parity of the operators. Studying the chiral properties of the scalar condensate with Wilson fermions, a similar suggestion was made by the authors in ref. [20]. In the special case of choosing $\omega = \pm\pi/2$, such an averaging procedure is done automatically. A change of the sign of r is equivalent to $\omega \to \omega + \pi$. Hence, for $\omega = \pm\pi/2$ all the quantities that are even under $\omega \to -\omega$ are automatically improved without any averaging procedure.

It is the aim of this paper to check this conjecture in practical simulations by performing a scaling test for the vector meson mass m_{V} and the pseudoscalar decay constant F_{PS} at $\omega = \pi/2$. The main goal is to test whether the results for m_{V} and F_{PS} are consistent with the anticipated leading $\mathrm{O}(a^2)$ behaviour and that the linear a dependence is indeed cancelled. In addition, it is an interesting and important question, what the size of the remaining lattice spacing effects arising in $\mathrm{O}(a^2)$ will be.

Let us list a few properties of the composite fields in the twisted mass formulation before going to the numerical results. Due to the transformation rule (2-2) one also has to transform the composite fields defined in the usual way,

$$\begin{aligned} S^0(x) &= \bar{\psi}(x)\psi(x), \quad P^\alpha(x) = \bar{\psi}(x)\gamma_5\frac{\tau^\alpha}{2}\psi(x), \\ A_\mu^\alpha(x) &= \bar{\psi}(x)\gamma_\mu\gamma_5\frac{\tau^\alpha}{2}\psi(x), \quad V_\mu^\alpha(x) = \bar{\psi}(x)\gamma_\mu\frac{\tau^\alpha}{2}\psi(x)\,. \end{aligned} \tag{2-8}$$

As an example we give here the relations for the axial and vector currents in the "physical basis" (primed quantities) and "the twisted basis" (unprimed quantities),

$$A_\mu'^\alpha = \begin{cases} \cos(\omega)A_\mu^\alpha + \epsilon^{3\alpha\beta}\sin(\omega)V_\mu^\beta & (\alpha = 1,2), \\ A_\mu^3 & (\alpha = 3), \end{cases} \tag{2-9}$$

$$V_\mu'^\alpha = \begin{cases} \cos(\omega) V_\mu^\alpha + \epsilon^{3\alpha\beta} \sin(\omega) A_\mu^\beta & (\alpha = 1,2), \\ V_\mu^3 & (\alpha = 3). \end{cases} \tag{2-10}$$

Note that in eq. (2-9) for $\alpha = 1, 2$ and $\omega = \pi/2$ the role of the axial and vector currents are just interchanged. Of particular interest is the PCVC relation, which takes the following form in the twisted basis:

$$\partial_\mu^* V_\mu^\alpha \;=\; -2\mu_q \epsilon^{3\alpha\beta} P^\beta \;, \tag{2-11}$$

where ∂_μ^* is the usual backward derivative. Through a vector variation of the action one obtains the point-split vector current as defined in [8, 16]. This current is protected against renormalisation and using the point-split vector current, the PCVC relation is an exact lattice identity. This implies that $Z_P = Z_\mu^{-1}$, where Z_μ is the renormalisation constant for the twisted mass μ_q. This will become important in the extraction of the pseudoscalar decay constant $F_{\rm PS}$ as described below.

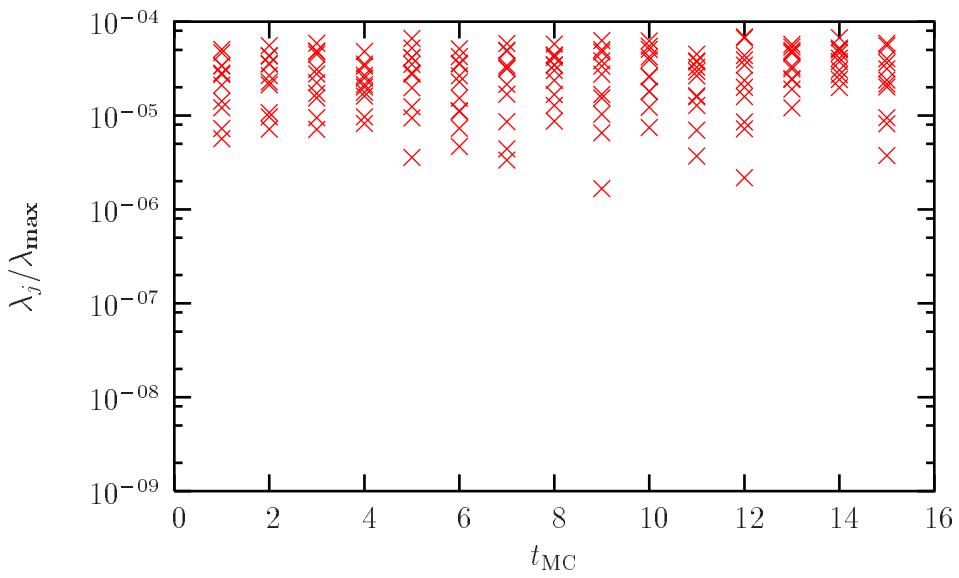
3 Numerical Tests

In this section, we describe our numerical results for testing the scaling behaviour of Wilson tmQCD in the quenched approximation. We started our investigation by performing a comparative benchmark study of different solvers for obtaining the quark propagator. We found the CGS algorithm [21] to be superior to the BiCGstab and the CG algorithms. We therefore used the CGS algorithm throughout this work. Gauge field configurations were generated by standard heat-bath and over-relaxation techniques.

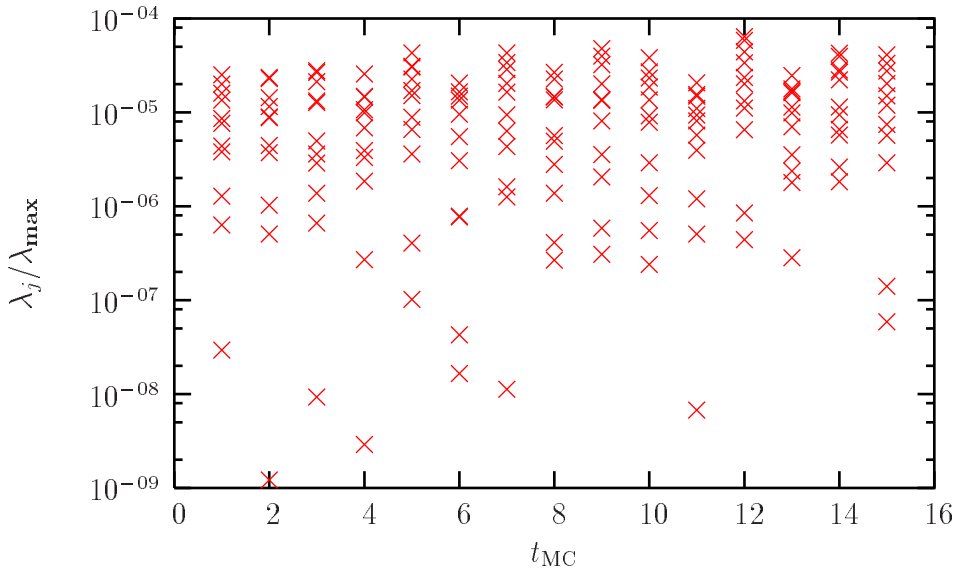
3.1 Mass average

In order to test the predictions of ref. [1], we started with the mass average procedure. To this end, we selected a value of $\beta = 5.85$, set the Wilson parameter $r = 1$ and performed simulations on $12^3 \times 24$ lattices at positive and negative values of $m_q = 1/2\ (1/\kappa - 1/\kappa_c)$. While for $m_q = +0.02725$, the propagator computations went smoothly, for $m_q = -0.02725$ the computation of the quark propagator was exceedingly expensive. The reason for this behaviour can be traced back to the spectrum of the Wilson tmQCD operator as can be seen in fig. 1.

Comparing fig. 1(a) with fig. 1(b), in the case of negative m_q one has to deal with extremely small eigenvalues of the operator $(D_W + m_0)^\dagger (D_W + m_0)$.



(a) $m_q = +0.02725, \kappa = 0.16025$



(b) $m_q = -0.02725, \kappa = 0.163099$

Figure 1: Monte Carlo time evolution of the eleven smallest eigenvalues λ of $(D_W + m_0)^\dagger (D_W + m_0)$, normalised by the largest eigenvalue, at $\mu_q = 0$ and $m_q = \pm 0.02725$ on a $12^3 \times 24$ lattice $(\kappa_c = 0.161662(17), \beta = 5.85)$.

Clearly, these very small low-lying eigenvalues lead to a poor convergence of the solver employed and hence to very costly simulations. Projecting out these small modes does also not help in this respect since the computation of the eigenvalues is again costly.

We therefore proceeded to the "self-averaging" case of choosing $\omega = \pi/2$, for which it has been shown in [1] that one gets $O(a)$ improvement even without the need of any averaging for all quantities that are even under $\omega \to -\omega$. In our practical implementation we have used the twisted basis. Hence, the choice $\omega = \pi/2$ corresponds to set $m_q = 0$ and $\mu_q \neq 0$. In this situation, the corresponding Wilson-Dirac operator is protected against small eigenvalues and we do not expect difficulties with the simulations.

3.2 Scaling of the vector meson mass

In order to verify the prediction of ref. [1] we computed the vector meson mass $m_{\rm V}$ and the pseudoscalar decay constant $F_{\rm PS}$ for the following values of β: 5.85, 6.0, 6.1, 6.2. We used periodic boundary conditions. The corresponding lattice volumes were $14^3 \times 28$, $16^3 \times 32$, $20^3 \times 40$ and $24^3 \times 48$, respectively.

For our simulation in the twisted basis at $m_0 = m_c$ we had to determine the critical hopping parameter κ_c for each value of β. At all the β values of our simulations we made our own determination of the value of κ_c from the intercept in κ at zero pion mass. The values of κ_c are given in table 1. Note that these critical values of κ have an intrinsic uncertainty of $O(a)$. This is, however, sufficient for obtaining fully $O(a)$ improved results in Wilson tmQCD [1].

β	L	T	$\kappa_{\rm c}$	μ_q	$N_{\rm meas}$
5.85	14	28	0.161662(17)	0.0376	400
6.0	16	32	0.156911(35)	0.03	388
6.1	20	40	0.154876(10)	0.025854	299
6.2	24	48	0.153199(16)	0.021649	215

Table 1: Parameters of the simulations. Note that the values for $\kappa_{\rm c}$ are obtained from a different set of measurements.

In order to fix the physical situation in our scaling test, we kept $r_0 m_{\rm PS}$ fixed for all values of β. For this purpose we determined the value of μ_q to fix $r_0 m_{\rm PS} = 1.79$. The corresponding values of μ_q for each value of β and all our simulation parameters are given in table 1.

We computed the standard 2-point correlation functions at zero momentum for the pseudoscalar and axial operators (which in the twisted basis at

$\omega = \pi/2$ gives the correct operator to extract the vector meson mass),

$$f_P^\alpha(t) = \sum_{\vec{x}} \langle P^\alpha(x) P^\alpha(0) \rangle \tag{3-1}$$

$$f_A^\alpha(t) = \frac{1}{3} \sum_{i=1}^{3} \sum_{\vec{x}} \langle A_i^\alpha(x) A_i^\alpha(0) \rangle \tag{3-2}$$

with $P^\alpha(x)$ and $A^\alpha(x)$ given in eqs. (2-8) and $x = (\vec{x}, t)$. In order to obtain a non-vanishing result, the flavour index has to be the same in these correlation functions and we will choose $\alpha = 1$ in the following. The pion mass could be extracted easily from the exponential decay of the correlation function $f_P^\alpha(t)$. For the vector meson mass, we performed two mass fits for the ground state mass and the first excited state. We checked the stability of the fit by changing the value of $t_{\rm min}$ where the fit started. As a cross check, we also determined the effective ground state mass and found consistent results. All errors were computed by a jackknife analysis. The numerical results at our simulation points are collected in table 2.

β	r_0/a	$am_{\rm PS}$	$am_{\rm V}$	$aF_{\rm PS}$
5.85	4.067	0.4340(16)	0.656(11)	0.1147(11)
6.0	5.368	0.3329(21)	0.488(11)	0.0859(9)
6.1	6.324	0.2871(17)	0.427(9)	0.0717(8)
6.2	7.360	0.2438(16)	0.363(10)	0.0640(10)

Table 2: Results for the vector meson mass and the pseudoscalar decay constant.

In fig. 2 we show our results for the vector meson mass as a function of a^2 represented by the open circles. In addition, we also show results from non-perturbatively O(a) improved Wilson fermions (filled circles) [13]. Finally, we added results for standard Wilson fermion simulations, see [12] and references therein, as they were available in the literature. We remark that the published data were not always at exactly the same value of $r_0 m_{\rm PS}$ that we used for our Wilson tmQCD simulations. In such cases we performed an interpolation to the desired value of $r_0 m_{\rm PS}$. The error from this (small) interpolation is negligible for the results presented here.

We performed a simple extrapolation of the Wilson tmQCD and the O(a) improved data of the form $r_0 m_{\rm V} = r_0 m_{\rm V}^{\rm cont} + b \cdot (a/r_0)^2$, with $r_0 m_{\rm V}^{\rm cont}$ the continuum value of the vector meson mass and $r_0 \simeq 0.5\,$fm. For the pure Wilson results we replaced the quadratic term with a term proportional to (a/r_0) in the extrapolation. Let us remark that our data for $m_{\rm V}$ for Wilson tmQCD has about a factor of four less statistics than the data from O(a)-improved

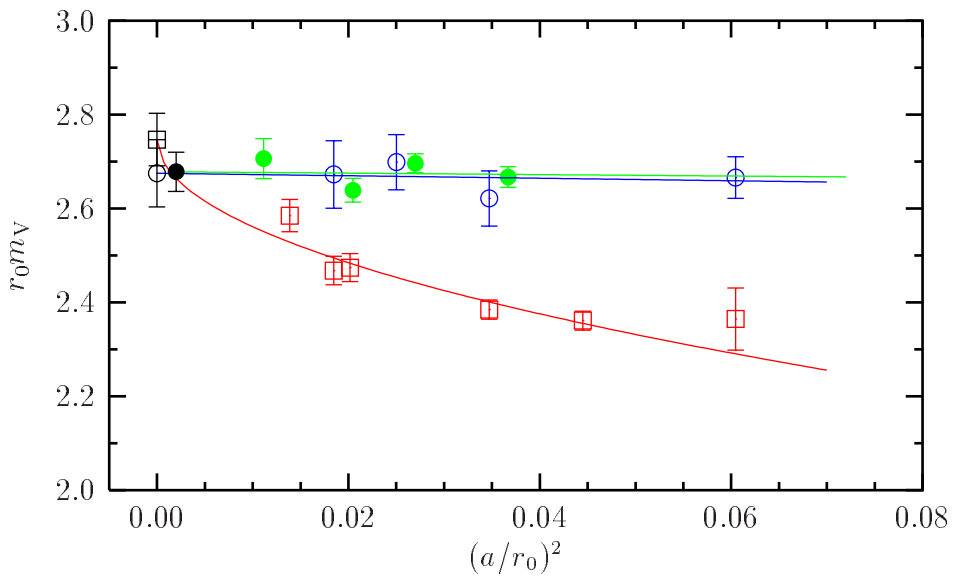


Figure 2: Scaling behaviour of the vector meson mass as a function of the lattice spacing squared for fixed pion mass, $r_0 m_{PS} = 1.79$. Open circles denote Wilson tmQCD, while filled circles are from non-perturbatively improved Wilson fermions [13]. The Wilson data without improvement (open squares) are collected from several sources in the literature. Note that the filled circles are slightly displaced for better visibility.

Wilson fermions, which is reflected in the larger error bars. Nevertheless, it is evident that the Wilson tmQCD results show a very similar scaling behaviour as the O(a)-improved Wilson fermions. This becomes even clearer when we compare with the unimproved pure Wilson data for m_V that we show as open squares in fig. 2. Here large lattice artefacts are seen and the scaling behaviour is much worse than with Wilson tmQCD or O(a)-improved Wilson fermions. We also note that the data for Wilson tmQCD are rather flat as a function of a^2 indicating that also higher order lattice spacing effects are suppressed. Clearly, it would be desirable to test these promising results in more precise simulations using a much higher statistics.

3.3 Scaling test for $F_{\rm PS}$

In order to extract the pion decay constant $F_{\rm PS}$ as another quantity to test scaling, we start with the standard definition of $F_{\rm PS}$ (again fixing the flavour index $\alpha = 1$),

$$\langle 0|A_0^1|PS\rangle = m_{\rm PS} F_{\rm PS} \ . \tag{3-3}$$

In the twisted basis, at $\omega = \pi/2$, the axial current is related to the vector current by the transformation eq. (2-2), see eqs.(2-9,2-10), and so we can write

$$\partial_\mu \langle 0|V_\mu^2|{\rm PS}\rangle = F_{\rm PS} m_{\rm PS}^2 \ . \tag{3-4}$$

Using the vector Ward identity in eq. (2-11), we can finally relate the divergence of the vector current to the pseudoscalar density and obtain

$$F_{\rm PS} m_{\rm PS}^2 = \partial_\mu \langle 0|V_\mu^2|{\rm PS}\rangle = 2\mu_q \langle 0|P^1|PS\rangle \ . \tag{3-5}$$

For asymptotic Euclidean times, the pseudoscalar correlation function f_P^1 assumes the form

$$f_P^1(t) = \frac{|\langle 0|P^1|{\rm PS}\rangle|^2}{2m_{\rm PS}} \cdot \left(e^{-m_{\rm PS} t} + e^{-m_{\rm PS}(T-t)}\right) \ , \ a \ll t \ll T \ . \tag{3-6}$$

Thus, by fitting the pseudoscalar correlation function for large time separations, we can obtain $m_{\rm PS}$ and the amplitude $|\langle 0|P^1|{\rm PS}\rangle|^2/m_{\rm PS}$ from which we then compute the desired matrix element $|\langle 0|P^1|{\rm PS}\rangle|$. Hence, we have all necessary ingredients to determine $F_{\rm PS}$ from eq. (3-5), without the need of any renormalisation factor, since $Z_P = Z_\mu^{-1}$, as we have mentioned in the previous section. The error estimate of the so computed value of $F_{\rm PS}$ is performed with a jackknife procedure. We note that the discussion of how to get $F_{\rm PS}$ with tmQCD resembles very closely the strategy one would follow in the continuum or with overlap fermions.

In fig. 3 we show our results for $r_0 F_{\rm PS}$ at a fixed value of $r_0 m_{\rm PS} = 1.79$. We also add results from O(a)-improved Wilson fermions [13] in the figure. We performed an extrapolation of the Wilson tmQCD and the O(a)-improved data of the form $r_0 F_{\rm PS} = r_0 F_{\rm PS}^{\rm cont} + b' \cdot (a/r_0)^2$, with $r_0 F_{\rm PS}^{\rm cont}$ the continuum value of the pion decay constant in units of $r_0 \simeq 0.5\,$fm. While the O(a)-improved Wilson results do show cut-off effects, presumably due to the particular value of the improvement coefficient c_A employed in these calculations, the results for Wilson tmQCD are essentially flat, indicating that also the higher order lattice spacing effects are substantially smaller.

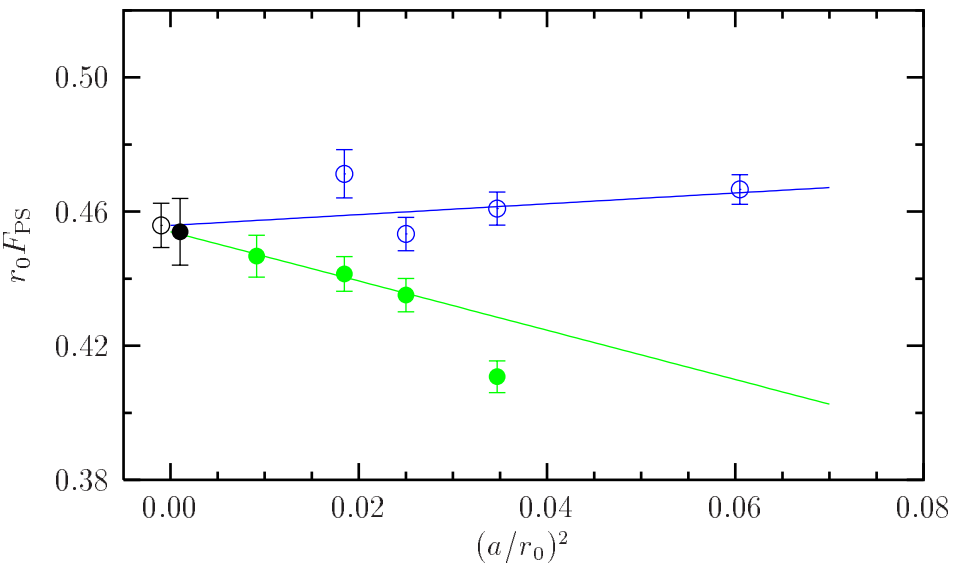


Figure 3: Scaling behaviour of the pion decay constant $F_{\rm PS}$ as a function of the lattice spacing for fixed pion mass, $r_0 m_{\rm PS} = 1.79$. Open circles denote Wilson tmQCD, while filled circles are from non-perturbatively improved Wilson fermions [13], for which only the three data points with smallest values of $(a/r_0)^2$ are included in the fit. Note that the points corresponding to the continuum extrapolation $F_{\rm PS}^{\rm cont}$ are slightly displaced for better visibility.

4 Conclusion and Outlook

In this paper we tested the striking idea of using the standard Wilson-Dirac operator with a twisted mass and twist angle $\omega = \pi/2$ to obtain full $\mathrm{O}(a)$ improvement for physical quantities that are even under $\omega \to -\omega$. The results of our – quenched – study for the vector meson mass m_{V} and the pion decay constant F_{PS} are very encouraging. It seems that in this setup the lattice spacing effects are substantially reduced with respect to standard Wilson fermions and consistent with vanishing $\mathrm{O}(a)$ discretisation errors. At the same time it seems that also lattice spacing effects that come in higher orders in a are small, a result that could not be anticipated before.

Thus it seems that Wilson twisted mass QCD has the potential to solve many problems at once:

- It automatically reduces lattice spacing effects, consistent with $\mathrm{O}(a)$ improvement.
- It protects against very small low-lying eigenvalues of the lattice Dirac operator.
- It can avoid unwanted phase transitions as appeared in dynamical simulations with clover improved Wilson fermions and Wilson gauge action.

In the light of this, dynamical simulations with twisted mass QCD appear to be very promising to approach the physical point at realistic values of quark masses. In some way, the twisted mass plays a similar role as an infrared cut-off as the quark mass in the staggered fermion or overlap approach does. The very good performance of staggered dynamical simulations gives hope that also in twisted mass QCD the simulations can be accelerated as compared to standard, improved or unimproved, Wilson fermions. Naturally, with Wilson twisted mass QCD the problem of unphysical taste degrees of freedom is completely avoided, which, to us, is a clear advantage of the tmQCD idea.

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