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Lattice Spacing Dependence of the First Order Phase Transition for Dynamical Twisted Mass Fermions

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Abstract

Lattice QCD with Wilson fermions generically shows the phenomenon of a first order phase transition. We study the phase structure of lattice QCD using Wilson twisted mass fermions and the Wilson plaquette gauge action in a range of β values where such a first order phase transition is observed. In particular, we investigate the dependence of the first order phase transition on the value of the lattice spacing. Using only data in one phase and neglecting possible problems arising from the phase transition we are able to perform a first scaling test for physical quantities using this action.

1 Introduction

Understanding the phase structure of lattice QCD is an important pre-requisite before starting large scale simulations. Indeed, our collaboration found that when working at lattice spacings of about 0.15 fm there can be strong first order phase transitions at small quark masses, at least when a combination of Wilson plaquette action and Wilson fermions is used [1, 2]. The phenomenon appears also when a small twisted mass term is switched on. This has serious consequences, since in such a scenario the pion mass $m_{\rm PS}$ cannot be made arbitrarily small but assumes a minimal value, $m_{\rm PS}^{\rm min}$, which may be about 500 MeV and hence it becomes impossible to work close to the physical value of the pion mass.

The presence of the first order phase transition for pure Wilson fermions is in accordance with predictions from chiral perturbation theory [3], which have been extended later to the case of adding a twisted mass [4, 5, 6, 7, 8]. Let us, for completeness, also mention that for values of the lattice spacing much coarser than $a = 0.15$ fm the first order phase transition turns into a second order one from the normal QCD phase to the so-called Aoki phase [9, 10, 11]. The generic phase structure of lattice QCD according to our present understanding is discussed and illustrated in refs. [1, 2, 12].

In refs. [1, 2] we have studied only one value of the inverse gauge coupling $\beta = 6/g_0^2$ in order to demonstrate the existence of the first order phase transition, leaving the question of the β dependence open. Since lattice chiral perturbation theory predicts a weakening of the first order phase transition towards the continuum limit, it is interesting to check this prediction and, in particular, to investigate quantitatively how fast the transition weakens when the continuum limit is approached. The answer to the latter question will naturally depend on the choice of the actions that are used for the gauge and the fermion fields.

In this paper we will present results using Wilson twisted mass fermions and the Wilson plaquette gauge action for three values of β. At each of these β values we have performed simulations at a number of quark masses on both sides of the first order phase transition. This allows to study the β dependence of the phase transition itself and, in addition, the lattice spacing dependence of physical observables computed separately in the two phases. We have performed such a scaling test for the pion mass, the pion decay constant and the ratio of the pion to the vector meson mass. For a scaling test of Wilson twisted mass fermions and other recent results in the quenched approximation see refs. [13, 14, 15].

2 Wilson twisted mass fermions

In this paper we will work with Wilson twisted mass fermions [16] that can be arranged to be $O(a)$ improved without employing specific improvement terms [17]. The Wilson tmQCD action in the twisted basis can be written as

$$S[U,\chi,\bar{\chi}] = a^4 \sum_x \bar{\chi}(x)(D_W + m_0 + i\mu\gamma_5\tau_3)\chi(x) \;, \tag{1}$$

where the Wilson-Dirac operator $D_{\rm W}$ is given by

$$D_{\rm W} = \sum_{\mu=0}^{3} \frac{1}{2}[\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a\nabla^*_\mu\nabla_\mu] \tag{2}$$

and ∇_μ and ∇^*_μ denote the usual forward and backward derivatives and the Wilson parameter r was set to 1.

The situation of full twist and hence automatic $O(a)$ improvement arises when m_0 in eq. (1) is tuned towards a critical bare quark mass $m_{\rm crit}$. We use for our simulations the hopping representation of the Wilson-Dirac operator with $\kappa = (2am_0 + 8)^{-1}$.

We extract the pseudo scalar mass $m_{\rm PS}$ and the vector meson mass $m_{\rm V}$ from the usual correlation functions:

$$\begin{aligned} C_{PP}(x_0) &= a^3 \sum_{\mathbf{x}} \langle P^+(x) P^-(0)\rangle \;, \\ C_{VV}(x_0) &= \frac{a^3}{3} \sum_{k=1}^{3} \sum_{\mathbf{x}} \langle V_k^+(x) V_k^-(0)\rangle \;, \end{aligned} \tag{3}$$

where we consider the local bilinears $P^\pm = \bar{\chi}\gamma_5\frac{\tau^\pm}{2}\chi$ and $V^\pm_\mu = \bar{\chi}\gamma_\mu\frac{\tau^\pm}{2}\chi$. Here we used $\tau^\pm = (\tau_1 \pm i\tau_2)$ with $\tau_{1,2}$ the first two Pauli matrices. Similarly one can define the correlation function C_{AP} with the local bilinear $A^\pm_\mu = \bar{\chi}\gamma_\mu\gamma_5\frac{\tau^\pm}{2}\chi$.

The bare pseudo scalar decay constant $f_\chi^{\rm PS}$ in the twisted basis can be obtained from (cf. [18, 19])

$$f_\chi^{\rm PS} = m_{\rm PS}^{-1}\, r_{AP}\, \langle 0|P^+(0)|\pi\rangle \;, \tag{4}$$

where the ratio

$$r_{AP} = \frac{\langle 0|A_0^+(0)|\pi\rangle}{\langle 0|P^+(0)|\pi\rangle} \tag{5}$$

β	$L^3 \times T$	$a\mu$	a [fm]
5.1	$12^3 \times 24$	0.013	0.200(2)
5.2	$12^3 \times 24$	0.010	0.160(4)
5.3	$16^3 \times 32$	0.008	0.138(8)

Table 1: Simulation points for Wilson plaquette gauge action. For the three values of β we give the lattice extent, the value for $a\mu$ and the value of the lattice spacing in fm, determined using $r_0 = 0.5$ fm at the reference point (see text), where $(r_0 m_{\rm PS})^2 = 1.5$.

can be extracted from the asymptotic behavior of

$$\frac{C_{AP}(x_0)}{C_{PP}(x_0)} = r_{AP}\ \tanh[m_{\rm PS}\,(T/2 - x_0)]\,. \tag{6}$$

The bare PCAC quark mass $m_\chi^{\rm PCAC}$ in the twisted basis can then be computed from the ratio

$$m_\chi^{\rm PCAC} = \frac{f_\chi^{\rm PS}}{2\,\langle 0|P^+(0)|\pi\rangle}\, m_{\rm PS}^2\,. \tag{7}$$

The sign of $m_\chi^{\rm PCAC}$ and $f_\chi^{\rm PS}$ is determined by the sign of r_{AP} and therefore, the corresponding values can be negative. One has to keep in mind that $m_\chi^{\rm PCAC}$ and $f_\chi^{\rm PS}$, since measured in the twisted basis, do not correspond to the physical quark mass and the physical pseudo scalar decay constant, respectively. While the quark mass is given by a combination of the (renormalized) values of $m_\chi^{\rm PCAC}$ and μ, the pseudo scalar decay constant can be computed by the help of $f_\chi^{\rm PS}$ and the twist angle, as long as $f_\chi^{\rm PS} \neq 0$ and the value of the twist angle is different from $\pi/2$.

Note that the purpose of the present paper is *not* to work at full twist nor to extract physical quantities, but rather to study the lattice spacing dependence of the first order phase transition. For the same reason, we also do not address the question of the choice of the critical quark mass in order to stay at full twist here, see refs. [15, 14] for recent quenched simulations addressing this point.

3 The phase transition as a function of the lattice spacing

In order to study the lattice spacing dependence of the phase transition we have chosen three values of β: $\beta = 5.1$, $\beta = 5.2$ and $\beta = 5.3$. We scaled the volumes and the values of μ such that the physical volume is larger than 2 fm, roughly constant and that $r_0\mu \approx 0.03$, where r_0 is the Sommer scale [20] fixed to be $r_0 = 0.5$ fm. Note that the value of r_0/a depends on the value of the quark mass and therefore we had to choose a reference value for r_0/a as will be explained below. The parameters are summarized in table 1.

In practice it turned out that a very direct way of detecting the presence of a first order phase transition in lattice QCD is to monitor the behavior of the plaquette expectation value $\langle P \rangle$, e.g. as a function of κ for fixed twisted mass parameter μ. In such a situation, starting at identical parameter values from "hot" (random) or "cold" (ordered) configurations, $\langle P \rangle$ can assume different, co-existing values. In fig. 1 we show $\langle P \rangle$ as a function of $1/(2\kappa)$ for the three values of β. The picture is typical for the behavior of a first order phase transition with meta-stable branches, one with a low value of $\langle P \rangle$ and one with a high value of $\langle P \rangle$. We will denote in the following these branches as high ("H") and low ("L") plaquette phases, respectively.

The β-dependence shows that the gap in the plaquette expectation value ΔP decreases substantially when moving from $\beta = 5.1$ ($a \approx 0.20$ fm) to $\beta = 5.3$ ($a \approx 0.12$ fm), which is presumably due to the mixing with the chiral condensate as discussed in [1]. One possible definition for the quantity ΔP is the difference between low and high phase plaquette expectation value at the smallest value of κ where a meta-stability occurs.

Let us remark that the first order phase transition exists also in the continuum limit at zero quark mass where the scalar condensate has a jump as a consequence of spontaneous chiral symmetry breaking. This means, of course, that in the continuum limit the phase transition occurs only for $\mu = 0$.

We give our simulation parameters, the statistics of the Monte Carlo runs and the results for $am_{\rm PS}$, $af_\chi^{\rm PS}$, $am_\chi^{\rm PCAC}$ and r_0/a in tables 4, 5 and 6.

The meta-stability phenomenon observed in $\langle P \rangle$ can also be seen in fermionic quantities. As an example, we show in fig. 2 the values of the PCAC quark mass as obtained in the branches with high and low plaquette expectation values of fig. 1 for the three values of β. Again we observe that with increasing β the gap between positive (low plaquette phase)

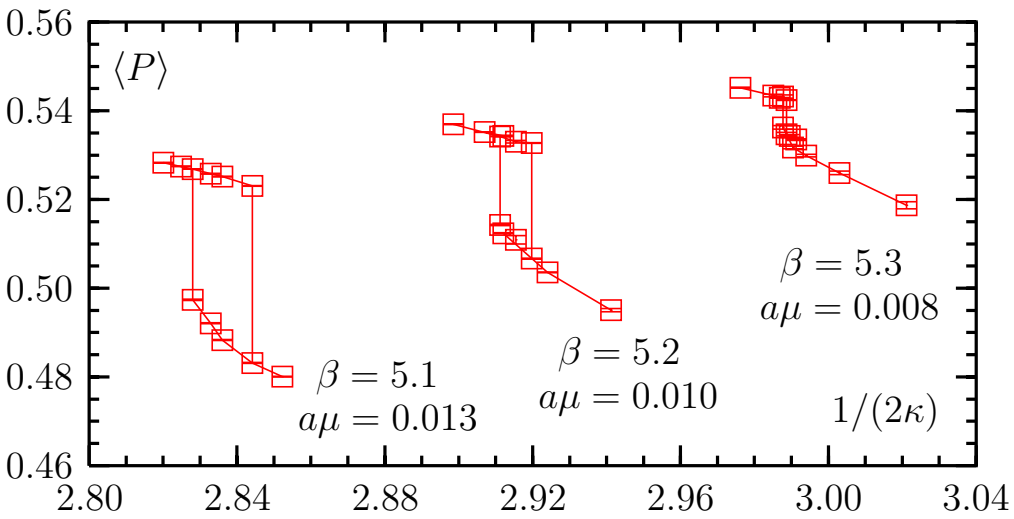

Figure 1: The plaquette expectation value $\langle P \rangle$ as a function of $1/(2\kappa)$ at the three values of β we have simulated. We also indicate the values of $a\mu$ which are scaled with β such that $r_0\mu$ is roughly constant. The lines just connect the data points and only serve to guide the eye. For this study we have more simulations points than in the next figures and than in tables 4, 5 and 6.

and negative (high plaquette phase) quark masses shrinks. Also, the meta-stability region in $1/(2\kappa)$ gets much narrower with increasing β.

The effects of the first order phase transition can also be seen in the pion mass and the value of the force parameter r_0. We plot in fig. 3 an example of the pion mass as a function of the PCAC quark mass at $\beta = 5.3$. The most intriguing observation here is that due to the presence of the first order phase transition, the pion mass, say for positive quark masses, does not go to zero but rather reaches a minimal value, and jumps then to the phase with negative quark mass. This is, of course, just another manifestation of the jump in the PCAC quark mass in fig. 2.

In fig. 4 we also show the values of r_0/a in the low and high plaquette phases at $\beta = 5.3$. Note that the values of r_0/a are quite different when determined in the low and the high plaquette phases, which is a generic feature also for other values of β and even for different gauge actions, see ref. [12].

An interesting question is, at which value of the lattice spacing a the minimal pion mass $m_{\rm PS}^{\rm min}$ assumes a value of, say, 300 MeV where contact to chiral perturbation could be established.

The pion mass assumes two different values for a fixed quark mass, once this quark mass

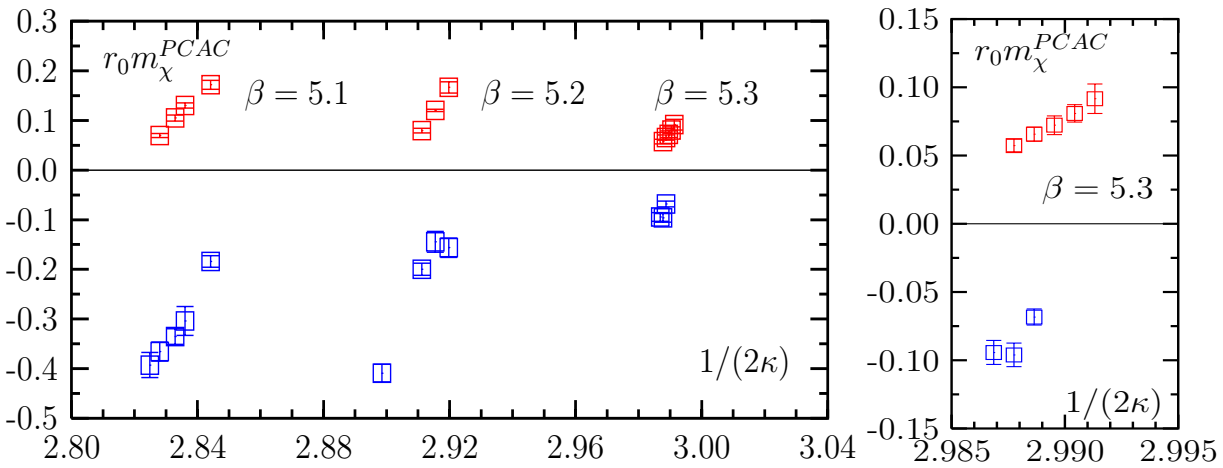

Figure 2: In the graph on the left the PCAC quark mass is plotted as a function of $1/(2\kappa)$ at the three values of β we have simulated. Positive values correspond to the low plaquette phase while negative values correspond to the high plaquette phase. The statistical errors are on this scale for most of the points smaller than the symbols. In the right plot we give a closeup of the $\beta = 5.3$ results.

β	$m_{\rm PS}^{\rm min}$[MeV]	ΔP
5.1	$\gtrsim 600$	0.0399(1)
5.2	$\gtrsim 630$	0.0261(1)
5.3	$\gtrsim 470$	0.0077(4)

Table 2: Minimal pion mass $m_{\rm PS}^{\rm min}$ in physical units in the low plaquette phase and ΔP for the three β values. To set the scale we used $r_0 = 0.5$ fm and the value of r_0/a measured for the corresponding simulation point.

lies inside the meta-stability region. These two values for the pion masses correspond to the two phases that for a certain interval of quark masses co-exist. The precise determination of the meta-stability region is, of course, very difficult. We can, however, give an interval in κ, $[\kappa_1, \kappa_2]$, that can be read from tables 4, 5 and 6 for the three different β values, where meta-stabilities occur in our simulation. In the following, we will mainly concentrate on the low plaquette phase since this is the natural choice for studying lattice QCD. Being interested only in the low plaquette phase we determine then a lower bound for the minimal pion mass as computed at the lower end of this interval, i.e. κ_1, in the low plaquette phase. We give in table 2 the values of the minimal pion masses in the low plaquette phase in physical units. In addition, we provide the value for the gap in the plaquette expectation value ΔP.

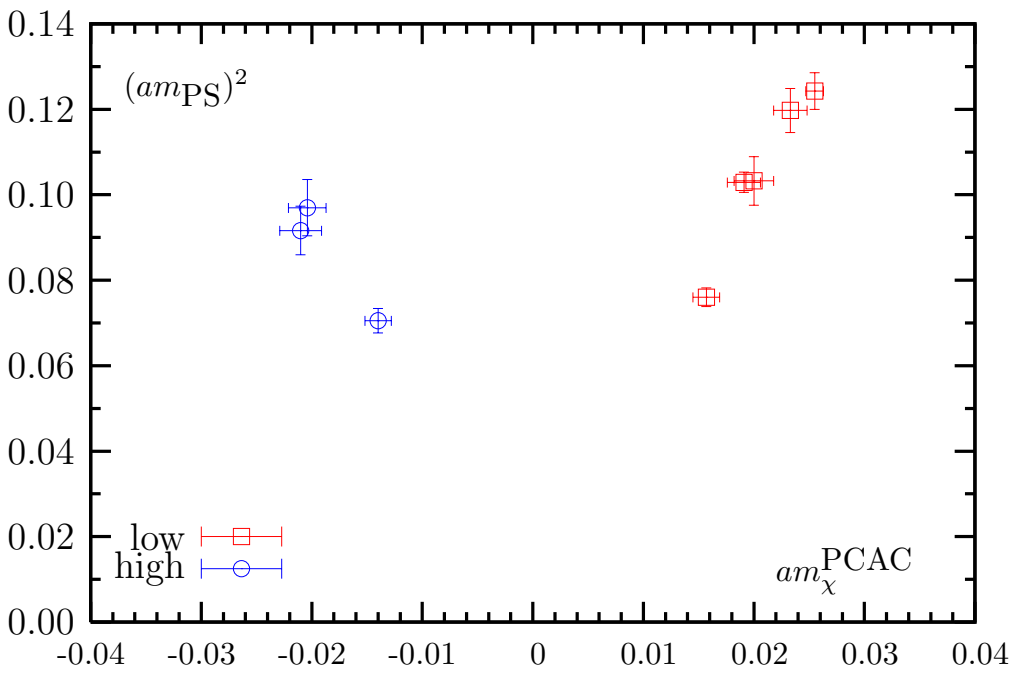

Figure 3: The squared pion mass as a function of the PCAC quark mass at $\beta = 5.3$.

In principle, it would be interesting to extrapolate the minimal pion mass and the gap in $\langle P \rangle$ as a function of the lattice spacing. However, our present data do not allow for a reliable and safe extrapolation. First of all, the determination of the minimal pion mass has a large ambiguity in itself since we do not know exactly for which value of the quark mass the meta-stability will disappear. A substantially larger statistics would be necessary to answer this question and to check whether tunneling from one phase to the other occurs. Second, the only three values of β we have used give a too short lever arm to perform a trustworthy extrapolation. And, third, the values of r_0/a are very different in the two phases, as can be seen in fig. 4, which makes it particularly difficult to follow the gap in $\langle P \rangle$ as a function of a/r_0.

Nevertheless, an estimate on a more qualitative level yields a value of the lattice spacing of $a \sim 0.07$ fm $- 0.1$ fm where simulations with pion masses of about 300 MeV can be performed without being affected by the first order phase transition.

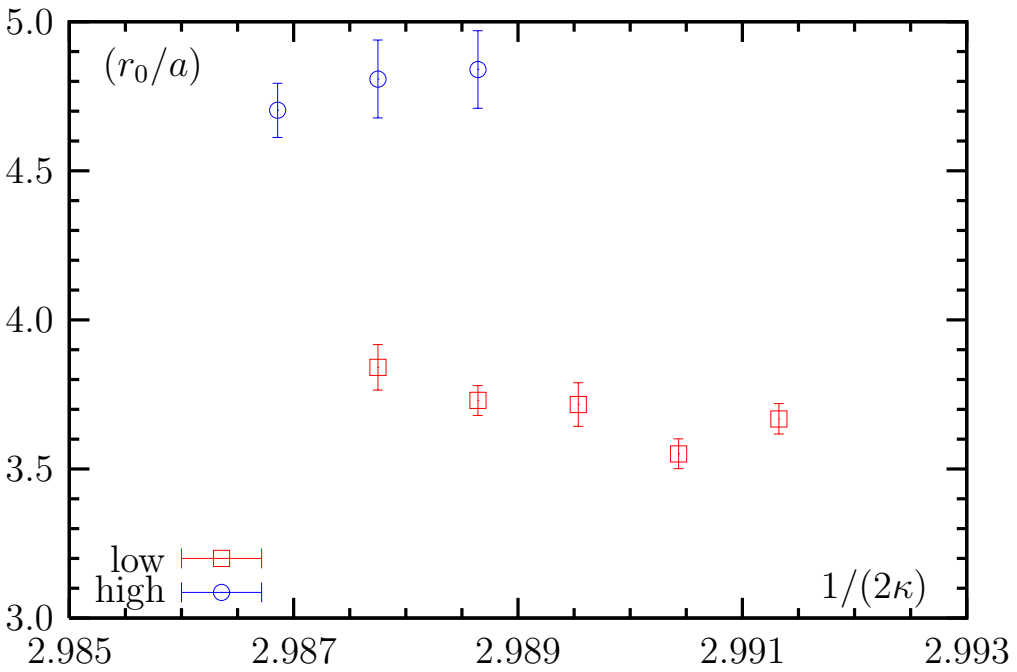

Figure 4: r_0/a as a function of $1/(2\kappa)$ at $\beta = 5.3$.

4 Lattice spacing dependence of physical observables

Although the present simulations are not at full twist, the fact that we have results at three values of β with roughly constant $r_0\mu$ allows us to check for the size of lattice artifacts. In order to perform such an investigation it is advantageous to express physical quantities in dimensionless variables. To this end, let us first define a reference pion mass through $(r_0 m_{\rm PS})^2 = 1.5$. We have chosen this particular value in order to be able to interpolate for the values of $\beta = 5.1$ and $\beta = 5.3$, and to perform only a short extrapolation for $\beta = 5.2$ to this point.

At the aforementioned reference pion mass, a corresponding reference value of r_0/a and a reference quark mass can be determined, the latter leading to a variable σ,

$$\sigma = \frac{m_\chi^{\rm PCAC}}{m_\chi^{\rm PCAC}\big|_{\rm ref}} \,. \tag{8}$$

β	$am_\chi^{\rm PCAC}\big\vert_{\rm ref}$	$af_\chi^{\rm PS}\big\vert_{\rm ref}$	$(r_0/a)\big\vert_{\rm ref}$
5.1	0.035(2)	0.195(06)	2.497(29)
5.2	0.025(4)	0.139(15)	3.124(85)
5.3	0.022(1)	0.122(07)	3.628(60)

Table 3: Reference values for $am_\chi^{\rm PCAC}$, $af_\chi^{\rm PS}$ and r_0/a. The reference point is chosen such that $(r_0 m_{\rm PS})^2 = 1.5$. The errors include the interpolation errors.

Similarly, we can define ratios for a quantity O,

$$R_O = \frac{O}{O\big\vert_{\rm ref}} \tag{9}$$

where $O|_{\rm ref}$ is the quantity as determined at the reference pion mass. The values for several quantities at the reference point can be found in table 3.

In order to determine the reference values for $m_\chi^{\rm PCAC}$, $f_\chi^{\rm PS}$ and r_0, in a first step we interpolated $m_\chi^{\rm PCAC}$ linearly as a function of $(r_0 m_{\rm PS})^2$ to the point where $(r_0 m_{\rm PS})^2 = 1.5$ and extracted the reference value for $m_\chi^{\rm PCAC}$. Then we determined the reference values for $f_\chi^{\rm PS}$ and r_0 by quadratically interpolating the data as a function of $m_\chi^{\rm PCAC}$ to the reference value of $m_\chi^{\rm PCAC}$. We repeated the latter step with a linear interpolation finding agreement within the errors. The fits to the data have been performed with the ROOT and MINUIT packages from CERN (cf. [21, 22]), taking the errors on both axis into account. We remark that for the quantity $r_0 m_{\rm PS}$ we have neglected the correlation of the data between r_0/a and $am_{\rm PS}$.

For a given observable O, R_O is a universal function of σ for fixed value of μ in physical units that allows for a direct comparison of results obtained at different values of β and, in principle, even for different actions. Deviations of results at different β values provide then a direct measure of scaling violations. In fig. 5 we show $R_{m_{\rm PS}^2}$ as a function of σ. Note that for the scaling analysis we take the data in the low plaquette phase only since this corresponds to the standard lattice QCD situation. We also remark that some of the points taken in this analysis might be meta-stable. Nevertheless, we assume here that these data can serve for checking scaling violations. Besides the data from the present work, we added also results from simulations at $\beta = 5.6$ [23], which were obtained, however, at vanishing twisted mass parameter $\mu = 0$.

A rather amazing consequence of fig. 5 is that, despite the fact that we are using coarse lattices, we cannot detect any scaling violation, at least within the (large) statistical errors

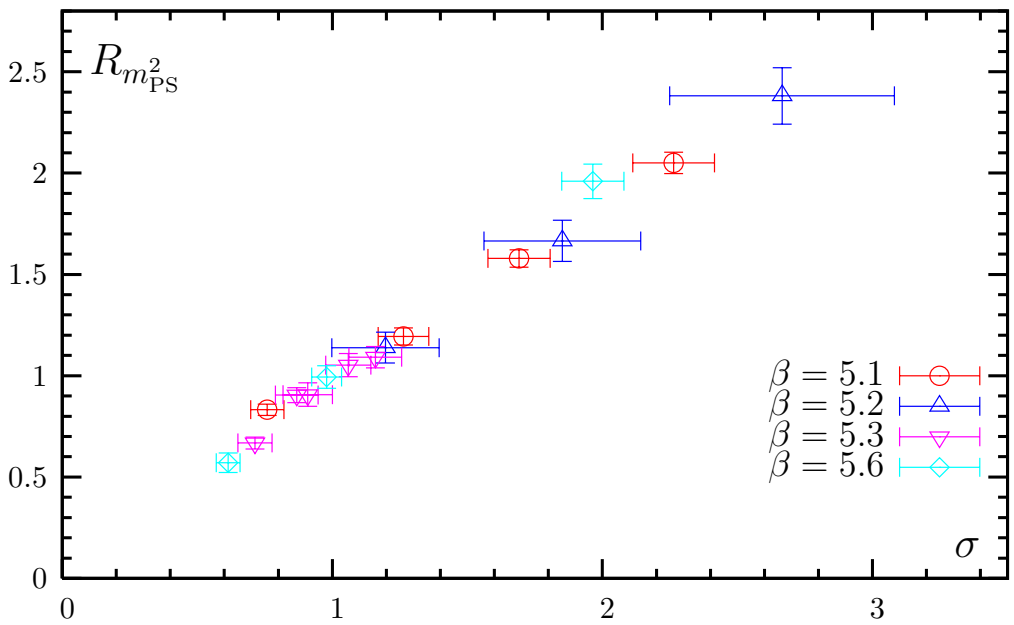

Figure 5: The dependence of the pion mass on the quark mass, i.e. $R_{m^2_{\rm PS}}$ as a function of σ. Besides the data of this work, we added in the plot also results from Wilson fermion simulations at $\beta = 5.6$ [23] which were obtained at $\mu = 0$.

of our data. Even more, the results of our present simulations at small values of β agree with results from simulations with pure Wilson fermions at $\beta = 5.6$ setting $\mu = 0$. The same observation is made for $R_{f^{\rm PS}_\chi}$, see fig. 6 and the ratio $m_{\rm PS}/m_{\rm V}$, see fig. 7. These results indicate that the lattice artifacts and the effect of a non-vanishing twisted mass parameter μ are surprisingly small. We remark here that in the case of the ratios like $R_{m^2_{\rm PS}}$ and $R_{f^{\rm PS}_\chi}$ one could have cancellation of mass independent cutoff effects. One has also to have in mind that, due to the presence of the first order phase transition, the simulated pion masses are still larger than 500 MeV. Whether our findings also hold when one is approaching the chiral limit is certainly an interesting but open question. However, in a set-up with Wilson twisted mass fermions and Wilson plaquette gauge action this question cannot be answered at these values of the lattice spacing.

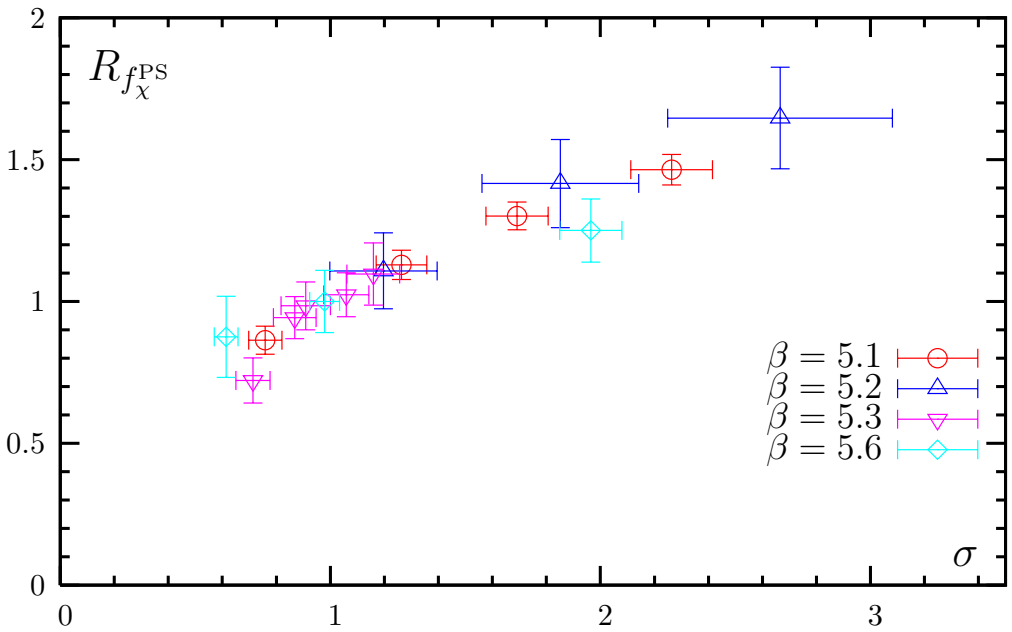

Figure 6: The ratio $R_{f_\chi^{\rm PS}}$ for the pseudo scalar decay constant as a function of σ. We also added results from Wilson fermion simulations for $R_{f_{\rm PS}}$ at $\beta = 5.6$ [23] obtained with $\mu = 0$.

5 Conclusions

In this paper we have investigated dynamical Wilson twisted mass fermions employing the Wilson plaquette gauge action. We have performed simulations at three values of $\beta = 5.1, 5.2, 5.3$, corresponding to values of the lattice spacing of $a \approx 0.20, 0.16, 0.14$ fm, respectively. The non-zero values of the twisted mass parameter μ were chosen such that $r_0\mu \approx 0.03$ for all of the three β values. At these rather coarse lattice spacings we find clear signals of first order phase transitions that manifest themselves in a meta-stable behavior of the plaquette expectation value and fermionic quantities, such as the PCAC quark mass and the pion mass.

We clearly observe that the gaps in quantities sensitive to the phase transition, such as the plaquette expectation value and the PCAC quark mass decrease substantially when β is increased. Unfortunately, with our present set of simulations, we are not able to quantitatively locate the value of the lattice spacing, where the effects of the first order phase transition becomes negligible and where a minimal pion mass of, say, 300 MeV can be reached. As an estimate of such a value of the lattice spacing we give a range of $a \approx 0.07$ fm $- 0.1$ fm.

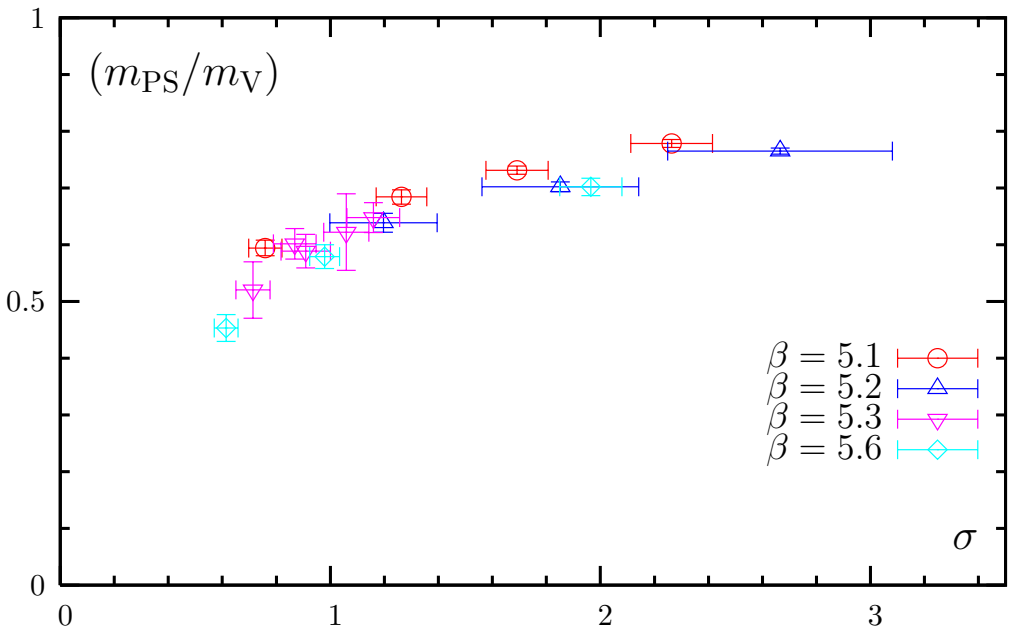

Figure 7: The ratio $m_{\rm PS}/m_{\rm V}$ as a function of σ. Again, we also added results from Wilson fermion simulations at $\beta = 5.6$ [23].

Of course, this would mean that a continuum extrapolation of physical results obtained on lattices with linear extent of at least $L = 2$ fm would be very demanding, since the starting point for such simulations would already require large lattices. It is therefore very important to find alternative actions such that the value of the lattice spacing can be lowered without running into problems with the first order phase transition. One candidate for such an action, the DBW2 gauge action, is discussed in ref. [12] where it has indeed been found that modifying the gauge action alone can substantially reduce the strength of the first order phase transition. We are presently investigating another possibility, the tree-level Symanzik improved gauge action [24, 25].

Despite the problems arising from the presence of a first order phase transition, we performed a scaling analysis for the pion mass, the pion decay constant and the ratio $m_{\rm PS}/m_{\rm V}$ for the data obtained at the three values of β where we performed simulations. To this end, we only analyzed data from the low plaquette phase, since this is the natural choice for QCD simulations.

By defining a reference pion mass at $(r_0 m_{\rm PS})^2 = 1.5$, we computed the ratio of $m_{\rm PS}$ and $f_\chi^{\rm PS}$ to the corresponding reference values as a function of the PCAC quark mass, again

measured with respect to the corresponding reference quark mass. We find that for these ratios the scaling violations are remarkably small and cannot be detected with the present precision of our data. Even more, when adding data from simulations of Wilson fermions with $\mu = 0$ at $\beta = 5.6$, then these data fall on the same scaling curve as our results on much coarser lattices and with twisted mass parameter switched on. This indicates that not only the lattice artifacts but also the effect of switching on a twisted mass of the order of $r_0\mu \approx 0.03$ are small, at least for the rather large pion masses simulated here. This finding is surprising since it suggests that continuum values of physical quantities can be already estimated from simulations at not too small lattice spacings. Of course, our scaling results suffer from the fact that they are obtained using data that might be meta-stable as a consequence of the presence of the first order phase transition. Hence, a scaling test with an action that does not lead to significant effects of the first order phase transition is mandatory to check the results presented in this paper.

6 Acknowledgments

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κ		$N_{\rm meas}$	$am_{\rm PS}$	$af_\chi^{\rm PS}$	$am_\chi^{\rm PCAC}$	r_0/a
0.1758	L	160	0.7015(031)	+0.2856(60)	+0.0799(12)	2.178(8)(4)(20)
0.1763	L	160	0.6155(040)	+0.2538(56)	+0.0597(12)	2.258(8)(0)(8)
0.1765	L	160	0.5353(068)	+0.2201(76)	+0.0446(16)	2.370(12)(4)(26)
0.1768	L	160	0.4468(051)	+0.1683(82)	+0.0268(13)	2.625(19)(22)(1)
0.1758	H	160	0.5323(126)	−0.2065(119)	−0.0496(25)	3.926(26)(12)(10)
0.1763	H	160	0.6771(116)	−0.2351(227)	−0.0777(50)	4.087(56)(4)(0)
0.1765	H	160	0.7231(111)	−0.2595(232)	−0.0864(26)	4.053(18)(17)(3)
0.1768	H	160	0.7377(119)	−0.2302(136)	−0.0926(38)	4.139(35)(16)(2)
0.1770	H	160	0.7530(189)	−0.2212(189)	−0.0977(59)	4.045(28)(10)(4)

Table 4: Parameters and physical observables for the simulations with $\beta = 5.1$. The lattice size in these runs was set to $12^3 \times 24$ and the twisted mass parameter to $a\mu = 0.013$. We give the values for κ and the number of measurements $N_{\rm meas}$ performed. We indicate with "L" or "H" whether the plaquette expectation assumes a low or a high value. Moreover, we give the values for $m_{\rm PS}$, $f_\chi^{\rm PS}$, $m_\chi^{\rm PCAC}$ and r_0 in lattice units. For r_0 we give in addition to the statistical error two systematic errors, the first of them coming from possible excited state contaminations and the second from the necessary interpolation of the force in r.

κ		$N_{\rm meas}$	$am_{\rm PS}$	$af_\chi^{\rm PS}$	$am_\chi^{\rm PCAC}$	r_0/a
0.17125	L	320	0.6057(025)	+0.2289(35)	+0.0650(08)	2.618(20)(5)(49)
0.17150	L	459	0.5066(050)	+0.1968(38)	+0.0452(08)	2.800(17)(9)(4)
0.17175	L	320	0.4189(071)	+0.1540(84)	+0.0292(17)	3.038(28)(14)(4)
0.17125	H	320	0.4173(111)	−0.1571(166)	−0.0352(43)	4.796(63)(65)(15)
0.17150	H	318	0.4220(126)	−0.1566(219)	−0.0349(50)	4.282(61)(16)(0)
0.17175	H	320	0.4985(088)	−0.1770(119)	−0.0494(28)	4.418(23)(23)(0)
0.17250	H	320	0.6462(131)	−0.1974(087)	−0.0874(24)	4.767(51)(7)(3)

Table 5: Parameter and physical observables for the simulations with $\beta = 5.2$. The lattice size in these runs was set to $12^3 \times 24$ and the twisted mass parameter to $a\mu = 0.01$. See table 4 for further explanations.

κ		$N_{\rm meas}$	$am_{\rm PS}$	$af_\chi^{\rm PS}$	$am_\chi^{\rm PCAC}$	r_0/a
0.16715	L	100	0.3525(061)	+0.1349(111)	+0.0255(18)	3.668(34)(9)(8)
0.16720	L	101	0.3460(075)	+0.1259(063)	+0.0233(15)	3.551(47)(2)(1)
0.16725	L	180	0.3213(088)	+0.1211(078)	+0.0200(18)	3.716(49)(24)(0)
0.16730	L	243	0.3208(037)	+0.1160(063)	+0.0191(15)	3.730(35)(6)(9)
0.16735	L	160	0.2757(040)	+0.0887(084)	+0.0157(12)	3.841(47)(28)(1)
0.16730	H	388	0.2656(054)	−0.1037(093)	−0.0140(12)	4.84(10)(2)(1)
0.16735	H	100	0.3114(106)	−0.1291(128)	−0.0204(17)	4.808(95)(33)(3)
0.16740	H	100	0.3027(094)	−0.1237(137)	−0.0210(19)	4.703(90)(0)(1)

Table 6: Parameter and physical observables for the simulations with $\beta = 5.3$. The lattice size in these runs was set to $16^3 \times 32$ and the twisted mass parameter to $a\mu = 0.008$. For further explanations see table 4.

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