Light quarks with twisted mass fermions

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Abstract

We investigate Wilson twisted mass fermions in the quenched approximation using different definitions of the critical bare quark mass $m_c$ to realize maximal twist and, correspondingly, automatic $O(a)$ improvement for physical observables. A particular definition of $m_c$ is given by extrapolating the value of $m_c$ obtained from the PCAC relation at non-vanishing bare twisted quark mass $\mu$ to $\mu = 0$. Employing this improved definition of the critical mass the Wilson twisted mass formulation provides the possibility to perform reliable simulations down to very small quark masses with correspondingly small pion masses of $m_\pi \simeq 250$ MeV, while keeping the cutoff effects of $O(a^2)$ under control.
1 Introduction

The combination of an automatic $O(a)$-improvement, the infrared regulation of small eigenvalues and fast dynamical simulations render the so-called twisted mass fermions [1, 2, 3] a most promising formulation of lattice QCD. There are already a number of results for the quenched approximation [4, 5, 6]. Also full QCD simulations with this approach have been performed and revealed a surprising phase structure of lattice QCD [7, 8]. On the theoretical side, extensive calculations in chiral perturbation theory were done [9, 10, 11].

One of the problems that appeared in the discussion of twisted mass fermions is the exact definition of the critical bare quark mass. In [12] it was shown that using the critical value of the bare quark mass where the pion mass vanishes, leads to a quark mass dependence of the pion decay constant $f_\pi$ that deviates strongly from the expected linear behavior. This "bending phenomenon" was observed when the quark mass $m_q$ obeys the inequality

$$am_q < a^2 \Lambda^2 .$$

The bending phenomenon was interpreted in a way that for such small values of the quark mass the Wilson term becomes the dominant term in the lattice Wilson-Dirac operator, thus leading to large lattice artefacts.

In refs. [13, 14] it has been suggested to take the value of the critical mass where the PCAC quark mass vanishes. In chiral perturbation theory it was demonstrated that this definition leads to a stable situation of "maximal twist" and hence to a reduction of lattice artefacts that otherwise would be enhanced at very small values of the quark mass. In refs. [15, 16] the theoretical background of such a definition is discussed on a general ground.

In this paper, we employ the definition of the critical mass by computing at non-zero twisted mass the critical hopping parameter as a functions of the twisted mass parameter and finally taking the limit to zero twisted mass. Such a definition is expected to eliminate large $O(a^2)$ artifacts at small values of the pion mass and should hence avoid the bending phenomenon. In the following we will shortly describe the encouraging results employing this improved definition of the critical mass. A more detailed scaling analysis of mesonic quantities will be reported elsewhere [17].

2 Wilson twisted mass fermions

In this paper we will work with Wilson twisted mass fermions that can be arranged to be $O(a)$ improved without employing specific improvement terms [1, 2]. The Wilson tmQCD action in the twisted basis can be written as

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

(2)
where the Wilson-Dirac operator $D_W$ is given by

$$D_W = \sum_{\mu=0}^{3} \frac{1}{2} [\gamma_{\mu}(\nabla_{\mu}^* + \nabla_{\mu}) - a \nabla_{\mu}^* \nabla_{\mu}]$$  \hspace{1cm} (3)$$

and $\nabla_{\mu}$ and $\nabla_{\mu}^*$ denote the usual forward and backward derivatives. We refer to [12] for further unexplained notations. The definition of the critical mass $m_c$ will be discussed in detail in the next section.

We extract pseudoscalar and vector meson masses from the correlation functions at full twist ($m_0 = m_c$):

$$C_P^a(x_0) = a^3 \sum_x \langle P^a(x) P^a(0) \rangle \quad a = 1, 2$$

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

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

where we consider the usual local bilinears $P^a = \bar{\psi} \gamma_5 \frac{\tau^a}{2} \psi$, $A_k^a = \bar{\psi} \gamma_k \gamma_5 \frac{\tau^a}{2} \psi$ and $T_k^a = \bar{\psi} \gamma_5 \frac{\sigma_{0k} \tau^a}{2} \psi$.

The untwisted PCAC quark mass $m_{PCAC}$ can be extracted from the ratio

$$m_{PCAC} = \frac{\sum_x (\partial_0 A_0^a(x) P^a(0))}{2 \sum_x \langle P^a(x) P^a(0) \rangle} \quad a = 1, 2$$  \hspace{1cm} (4)$$

Using the PCAC relation we can also compute the pion decay constant at maximal twist without requiring any renormalization constant (see [18, 4]):

$$f_\pi = \frac{2\mu}{(M_\pi)^2} |\langle 0 | P^a | \pi \rangle| \quad a = 1, 2$$  \hspace{1cm} (5)$$

3 Definition of the critical mass

The Wilson tmQCD action of eq. [2] can be studied in the full parameter space $(m_0, \mu)$. A special case arises, however, when $m_0$ is tuned towards a critical bare quark mass $m_c$. In such, and only in such a situation, all physical quantities are, or can easily be, $O(a)$ improved. The critical quark mass, or alternatively the critical hopping parameter $\kappa_c = \frac{1}{2am_c+s}$, has thus to be fixed in the actual simulation to achieve automatic $O(a)$-improvement at maximal twist.

In general, the definition of the critical mass has an intrinsic uncertainty that comes at $O(a)$ for Wilson fermions. This could be improved to an $O(a^2)$ uncertainty by using Clover fermions. If a definition of $\kappa_c$ from a linear extrapolation of $(m_\pi a)^2 \to 0$ is used, one has in addition an unrelated systematic error coming from
the long way of extrapolation from large pion masses of O(600 MeV).

A better definition of $\kappa_c$ can be obtained by the following procedure:

- At fixed non-zero twisted mass parameter the hopping parameter $\kappa_c(\mu a)$ is determined as the point where the PCAC quark mass of eq. (4) vanishes. The non-zero value of the twisted mass allows a safe interpolation in this case.

- As a further step, an only short linear extrapolation of $\kappa_c(\mu a)$ from small values of $\mu a$ to $\mu a = 0$ yields a definition of $\kappa_c$ which is expected [15, 16] to lead to small lattice artefacts, in particular also at small quark masses much below values indicated in the inequality of eq. (1).

In figure 1 we show an example of this extrapolation at $\beta = 5.7$, where we also indicate the $\kappa_c$-value determined by the vanishing pion mass squared.

![Figure 1: Determination of the critical mass: $1/\kappa_c$ versus $\mu a$ at $\beta = 5.7$, extrapolation to $\mu a = 0$, the open diamond indicates the $1/\kappa_c$ value determined by $(m_\pi a)^2 \to 0$ at $\mu = 0$ for unimproved Wilson fermions.](image)

The possible choices for the determination of the critical bare quark mass were also discussed in chiral perturbation theory [13, 14]. Recently, a definition of maximal twist from parity conservation has also been investigated in [8]. There, however, the critical masses $m_c(\mu a)$ were not extrapolated to $\mu a = 0$, but were used at the respective twisted mass parameter at which they were determined.
4 Numerical results

In this section we will provide a comparison of Wilson twisted mass results for the pion mass, the pion decay constant and the $\rho$-mass obtained with two different definitions of $\kappa_c$. The first, “pion mass” definition, refers to the limit $(m_\pi a)^2 \to 0$ taken at $\mu a = 0$. The second, “PCAC quark mass” definition, corresponds to the determination of $\kappa_c(\mu a)$ at fixed $\mu a \neq 0$ from the vanishing of the PCAC quark mass, $am_{PCAC}(\mu a)$ and then taking the limit $\kappa_c(\mu a \to 0)$. The latter $\kappa_c$ values were determined on a subset of $O(150)$ configurations for three couplings, namely $\beta = 5.70, 5.85$ and 6.0. The simulations were performed for a number of bare quark masses in a corresponding pion mass range of $250 \text{ MeV} < m_\pi < 1200 \text{ MeV}$ using a multiple mass solver [19] on $O(400)$ gauge field configurations generated with the Wilson plaquette gauge action.

In general the time component of the tensor correlator provides a better signal for the vector meson mass compared to the axial-vector correlator at maximal twist. This observation was made independently in [6] and is manifest in the smaller error bars displayed in figures of this section.

![Figure 2: Comparison of results at $\beta = 6.0$ for the pion mass for different definitions of the critical mass.](image)

The first quantity we investigated was the pion mass. In figure 2 we show the behavior of $(m_\pi a)^2$ versus $\mu a$ for the two definitions of $\kappa_c$. The results for the PCAC quark mass definition show a linear behavior down to very small bare quark masses,
while a small non-zero value is approached in the chiral limit with the pion mass
definition of $\kappa_c$. This residual $O(a)$ pion mass at $\mu a = 0$ can be attributed to the
$O(a)$ error in the critical mass determined by the vanishing of the pion mass in the
pure Wilson case.

At $\beta = 5.7$ (lattice size $12^3 \times 32$, $a \approx 0.17$ fm) we computed correlation functions
also for a third, intermediate definition of the critical mass: we chose the point where
the PCAC quark mass vanishes at small, but non-zero value of the twisted mass. In figure 3 we show the results for the pion decay constant and the vector meson
mass. It is obvious that already this intermediate definition of $\kappa_c$ substantially
diminishes the bending tendency of the data when approaching the chiral limit. Such
a definition of the critical hopping parameter $\kappa_c(\mu_0 a \neq 0)$ seems to be sufficient to
eliminate the deviation from a linear behavior for all twisted mass values $\mu a \geq \mu_0 a$.
The results for $\kappa_c(\mu a = 0)$ from the PCAC quark mass definition show a straight
behavior for both observables down to pion masses of about 250 MeV. The bending
phenomena reported in [12] can thus be attributed to the pion mass definition of
the critical mass in this simulation. Note that at $\beta = 5.7$ we are working at a rather
course value of the lattice spacing.

At $\beta = 5.85$ (lattice size $16^3 \times 32$, $a \approx 0.12$ fm) we can now compare our previous
and new Wilson twisted mass results with the data from overlap fermion simulations
[12] which were obtained on a smaller lattice volume ($12^3 \times 24$). Using the definition
of $\kappa_c$ from the vanishing of the PCAC quark mass, the bending near the chiral limit
vanishes almost completely both for the pion decay constant and the vector meson
mass extracted from the tensor correlator (see figure 4). In both cases the overlap
fermion results lie slightly higher than the twisted mass fermion results. This fact
might be explained by residual finite volume effects and/or different lattice artefacts.

Finally we show in figure 5 the results at $\beta = 6.0$ (lattice size $16^3 \times 32$, $a \approx
0.09$ fm). Although the physical volume is smaller than the one at $\beta = 5.85$ we are
able to confirm the absence of bending for small masses when using the PCAC quark
mass definition of $\kappa_c$. For the pion decay constant we observe a very good agreement
with the overlap fermion results of ref. [20] and with the twisted mass results using
the parity conservation definition of the critical mass from ref. [6]. For the vector
meson mass we refrain from comparing with the parity conservation definition, since
the error bars would cover both our results with the pion mass and PCAC quark
mass definition of the critical mass.

5 Conclusions

We have studied Wilson twisted mass fermions with different definitions of the critical mass. The "bending phenomena" in basic observables like the vector meson
mass and the pion decay constant using the critical mass from vanishing pion mass
at $\mu a = 0$ reported in [12] is absent for the choice of $\kappa_c$ from the vanishing of the
PCAC quark mass in the limit $\mu a \to 0$. This is true even at small values of the
pion mass close to the experimentally measured value where maybe contact to chiral perturbation theory can be made.

In ref. [6], the same definition of the critical mass has been employed, but at fixed twisted mass parameter separately at each simulation point. The results of this reference taken together with the findings in the present paper lead to the conclusion that the PCAC quark mass definition of the critical hopping parameter is a crucial element of twisted mass simulations in order to keep $O(a^2)$ effects well under control at small quark masses. This conclusion is in accordance with theoretical considerations [13, 14, 15, 16].

Employing the PCAC quark mass definition of the critical mass the Wilson twisted mass formulation provides the possibility to perform reliable simulations at very small quark masses ($m_\pi \simeq 250$ MeV). Thus, Wilson twisted mass fermions can be used to explore really light quarks on the lattice - as light as with overlap fermions, but at considerably lower cost (see [21] for a detailed cost comparison). This opens a very promising prospect for dynamical fermion simulations and renders twisted mass fermions as a real alternative to staggered fermions without the conceptual difficulties of the latter.

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Figure 3: Comparison of results at $\beta = 5.70$ for the pion decay constant (top) and vector meson mass (bottom) for different definitions of the critical mass.
Figure 4: Comparison of overlap fermion and Wilson twisted mass results at $\beta = 5.85$ for the pion decay constant (top) and vector meson mass (bottom) for different definitions of the critical mass.
Figure 5: Comparison of results at $\beta = 6.0$ for the pion decay constant (top) and vector meson mass (bottom) for different definitions of the critical mass.