Parton Distribution Functions
with Twisted Mass Fermions

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Abstract

We present a first Wilson twisted mass fermion calculation of the matrix
element between pion states of the twist-2 operator, which is related to the
the lowest moment $\langle x \rangle$ of the valence quark parton distribution function in a
pion. Using Wilson twisted mass fermions in the quenched approximation we
demonstrate that $\langle x \rangle$ can be computed at small pseudoscalar meson masses
down to values of order 250 MeV. We investigate the scaling behaviour of this
physically important quantity by applying two definitions of the critical mass
and observe a scaling compatible with the expected $O(a^2)$ behaviour in both
cases. A combined continuum extrapolation allows to obtain reliable results
for $\langle x \rangle$ at very small pseudoscalar meson masses, which previously could not
be explored by lattice QCD simulations.

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1 Introduction

In lattice QCD the so-called chiral extrapolation of data obtained at pseudoscalar meson masses of about 500 MeV to the physical pion mass value (140 MeV) is one of the main systematic uncertainties in today’s lattice QCD calculations. As an example from our own work let us quote a recent paper [1] where the lowest moment \( \langle x \rangle \) of the valence quark parton distribution function in a pion has been calculated, fully controlling the continuum limit, finite size effects [2] and the non-perturbative renormalization [3]. The only remaining uncertainty, besides the quenched approximation, was the chiral extrapolation.

In this letter we want to report on a first step towards eliminating also this systematic error by employing the twisted mass formulation of lattice QCD [4] which allows to regulate unphysically small eigenvalues of the Wilson-Dirac operator and simultaneously achieves an O(\( a \))-improvement of physical observables without the need of improvement coefficients [5] (automatic O(\( a \)) improvement). With the example of \( \langle x \rangle \) we will demonstrate that indeed this formulation of lattice QCD allows to bridge the gap between results at pseudoscalar meson mass values of 500 MeV or larger – as obtained in conventional simulations – and the physical value of the pion mass. Performing the simulations at a number of values of the gauge coupling \( g_0^2 = 6/\beta \), the continuum limit of \( \langle x \rangle \) is performed at values of the pseudoscalar meson mass small enough to allow, at least in principle, the comparison of the numerical results with the predictions from chiral perturbation theory.

Wilson twisted mass fermions have been employed already in a number of quenched simulations [6, 7, 8, 9, 10, 11, 12, 13, 14]. See refs. [15, 16] for recent reviews.

Also full QCD simulations using this approach have been performed and proved to be very useful in studying the phase structure of lattice QCD with Wilson type fermions [17, 18, 19, 20]. On the theoretical side, various studies were performed by means of the Symanzik expansion and of chiral perturbation theory [21, 22, 23, 24, 25, 26, 27].

In recent quenched simulations [10, 11, 12] it has been shown that the Wilson twisted mass approach can be used to simulate small pseudoscalar meson masses of order 250 MeV while keeping O(\( a^2 \)) cut-off effects under control, when employing the definition of the critical mass derived from the vanishing of the PCAC quark mass [25, 26, 27]. These simulations were done for basic observables as extracted from 2-point correlation functions. In this letter we will extend the investigation of Wilson twisted mass fermions also to the physically important case of 3-point functions, in particular for matrix elements related to moments of parton distribution functions which are relevant in deep inelastic scattering.
2 Lattice action and operators

2.1 Wilson twisted mass fermions

In this letter we will work on a lattice $L^3 \times T$ with Wilson twisted mass fermions [4] which can be arranged to be $O(a)$ improved without employing specific improvement terms [5]. The action for a degenerate flavour doublet of twisted mass fermions can be written as

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

where the Wilson-Dirac operator $D_W$ is given by

$$D_W = \sum_{\mu=1}^4 \frac{1}{2}[\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a \nabla^*_\mu \nabla_\mu] \quad (2)$$

$\nabla_\mu$ and $\nabla^*_\mu$ denote the usual forward and backward derivatives, $m_0$ and $\mu$ denote the untwisted and twisted bare quark masses. We refer to refs. [7, 8] for further unexplained notations. Here and in the following $\psi(x)$ indicates a flavour doublet of quarks.

A key element in this twisted mass setup is the definition of the critical quark mass $m_c$, since, in order to obtain automatic $O(a)$ improvement, the target continuum theory should have a vanishing untwisted quark mass. In the present work, we will employ two definitions for the critical mass with the final aim of a combined continuum extrapolation of the results obtained in the two cases. The first definition of the critical mass is the point where the pseudoscalar meson mass, computed with plain Wilson fermions ($\mu = 0$) vanishes, the second, where the PCAC quark mass, computed in the Wilson twisted mass setup, vanishes. See refs. [11, 11, 16], for details on how the critical mass has been computed numerically. In the following we will refer to the first situation as the “pion definition” and to the second situation as the “PCAC definition” of the critical point. Both definitions should lead to $O(a)$-improvement, but they can induce very different $O(a^2)$ effects, in particular at small pseudoscalar meson masses [25, 26, 27]. Indeed, in refs. [7, 8] we reported that the pion definition can have substantial $O(a^2)$ effects which are amplified when the quark mass becomes small and violates the inequality $\mu > a \Lambda^2$ (where $\mu$ is, at full twist, the parameter which provides mass to the pseudoscalar meson). On the other hand, when the PCAC definition of the critical mass is used, these particular kind of $O(a^2)$ cut-off effects are dramatically reduced as was shown numerically in refs. [10, 11, 12], and theoretically in refs. [25, 26, 27].

The purpose of the present letter is a demonstration that Wilson twisted mass fermions are in a position to reach small quark masses and eventually allow a comparison with chiral perturbation theory also for more complicated physical observables than the 2-point functions considered in refs. [3, 7, 8, 10, 11, 12, 13, 14].
computation of pion form factors employing the twisted mass fermion approach was already presented in ref. [9], but at a rather high values of the pseudoscalar meson mass (470 and 660 MeV), using only the pion definition of the critical quark mass.

2.2 The twist-2, non-singlet operator

The towers of twist-2 operators related to the unpolarized structure functions have the following expressions

\[ O_{a,\mu_1\cdots\mu_N}(x) = \frac{1}{2^{N-1}} \bar{\psi}(x) \gamma_{\mu_1} \tilde{D}_{\mu_2} \cdots \tilde{D}_{\mu_N} \frac{1}{2} \tau^a \psi(x) , \]  \hspace{1cm} (3)

where \{\cdots\} means symmetrization on the Lorentz indices and

\[ \tilde{D}_\mu = \bar{D}_\mu - D_\mu; \quad D_\mu = \frac{1}{2} \left[ \nabla_\mu + \nabla^*_\mu \right] . \]  \hspace{1cm} (4)

The flavour structure is specified by the Pauli matrices \( \tau^a \) where we include here also the identity with \( \tau^0 = 2 \cdot 1 \). In general one should perform an axial rotation in order to obtain the expressions for the twist-2 operators for the twisted mass formulation. For our purposes it is enough to notice that the operators in eq. (3) with flavour index \( a = 0, 3 \) do not rotate. We concentrate in this work on the twist-2 quark operator related to the lowest moment of the valence quark parton distribution function in a pion. In particular for the up quark (the down quark can be treated in the same way) this amounts to consider operators of the following form

\[ O^u_{\mu\nu}(x) = \frac{1}{2} \bar{\psi}(x) \gamma_{\mu} \tilde{D}_{\nu} \frac{1}{2} \left[ \gamma^4 \sum_{k=1}^{3} \gamma_k \tilde{D}_k \right] (1 + \tau^3) \psi(x) - \delta_{\mu\nu} \cdot \text{trace terms} , \]  \hspace{1cm} (5)

There are two representations of such a non-singlet operator on the lattice [28, 29]. In the following we will concentrate on the operator

\[ O_{44}^u(x) = \frac{1}{2} \bar{\psi}(x) \left[ \gamma_4 \tilde{D}_4 - \frac{1}{3} \sum_{k=1}^{3} \gamma_k \tilde{D}_k \right] \frac{(1 + \tau^3)}{2} \psi(x) , \]  \hspace{1cm} (6)

since in computing the matrix elements of this operator one has not to supply an external momentum (an external momentum increases considerably the noise to signal ratio).

The matrix elements of this operator can be computed in the standard way, described in refs. [30, 31]. We indicate with

\[ P^{\pm}(x) = \bar{\psi}(x) \gamma_5 \frac{\tau^\pm}{2} \psi(x) , \quad \tau^\pm = \frac{\tau^1 \pm i \tau^2}{2} \]  \hspace{1cm} (7)

the interpolating operator for the charged pseudoscalar meson. The ratio of the 3-point function

\[ C_{44}(y_4) = a^6 \sum_{x,y} \langle P^+(0) O_{44}(y_4) P^-(x, T/2) \rangle , \]  \hspace{1cm} (8)
and the 2-point function

\[ C_P(x_4) = a^3 \sum_x \langle P^+(0) P^-(x, x_4) \rangle, \tag{9} \]

is related to the matrix element we are interested in. The Wick contractions of the correlation function contain also a disconnected piece that we neglect consistently with the fact that we are interested in the valence quark distribution. In particular if we perform a transfer matrix decomposition and define

\[ R(y_4) = \frac{C_{44}(y_4)}{C_P(T/2)}, \tag{10} \]

in the limit when only the fundamental state dominates \( (0 \ll y_4 \ll T/2) \), and the ratio \( R \) reaches a plateau in \( y_4 \), we obtain

\[ \langle 0, PS|O_{44}|0, PS \rangle = 2m_{PS}R. \tag{11} \]

where \( |0, PS \rangle \) indicates the fundamental state in the charged pseudoscalar channel. The relevant bare quantity is then

\[ \langle x \rangle_{\text{bare}} = \frac{1}{m_{PS}} \cdot R. \tag{12} \]

In fig. we show an example of such a plateau from which we read off the bare matrix element, from our second smallest pseudoscalar meson mass and smallest lattice spacing.

The matrix element obtained in this way has to be renormalized by a multiplicative renormalization factor. To this end, we took the \( Z_{\text{RGI}} \) as computed in refs. \([1, 3]\) from a Schrödinger functional (SF) renormalization scheme \([32, 33, 34, 35]\), with standard Wilson action. The renormalization factor will affect the renormalized matrix element by \( O(a) \) contributions. In order to check the \( O(a) \) effects coming from the boundaries of the SF we have varied the improvement coefficients typical of the SF boundaries and we have observed no variation in the continuum limit, indicating that these boundary \( O(a) \) effects are negligible. Nevertheless the continuum limit discussed in the following section is always performed with the boundary improvement coefficients set to their perturbative values.

The renormalized matrix element has a well defined continuum limit and in the phenomenologically relevant \( \overline{\text{MS}} \) scheme it is given by

\[ \langle x \rangle_{\overline{\text{MS}}}^{\text{MS}}(\mu, r_0 m_{PS}) = \lim_{a \to 0} \frac{\langle x \rangle_{\text{bare}}(a, m_{PS}) Z_{\text{RGI}}(a)}{f_{\overline{\text{MS}}}(\mu)} \mu = 2 \text{ GeV}, \tag{13} \]

where \( Z_{\text{RGI}} \) and \( f_{\overline{\text{MS}}}(\mu) \) were computed in ref. \([\text{ I}]\) (see this reference for further details). We remind here that this \( \mu = 2 \text{ GeV} \) indicates the renormalization scale and not the twisted mass, since we are using a mass independent renormalization scale.
Figure 1: $\langle x \rangle^\text{bare}$ at $\beta = 6.2$ and a pseudoscalar meson mass of about 370 MeV; we show the average of the two plateaux around $T/4$ and $3T/4$.

3 Numerical results

Our quenched simulations were performed for a number of bare quark masses in a corresponding pseudoscalar meson mass range of $270 \text{ MeV} < m_{PS} < 1.2 \text{ GeV}$ using the Wilson plaquette gauge action, employing periodic boundary conditions for all fields. In table 1 we give further details of our simulation parameters.

We performed simulations at different values of the twisted mass parameter $\mu$ while setting $m_0$ to its critical value as obtained from the pion or the PCAC definition. The corresponding critical hopping parameters can be found in ref. [12]. The results are summarized in table 2 for the pseudoscalar mass and in table 3 for the bare matrix element.

The goal of this letter is to perform the continuum extrapolation of $\langle x \rangle$ at a fixed value of $m_{PS} r_0$, for a number of values of $m_{PS} r_0$. An interpolation of the values of $\langle x \rangle$ to the chosen values of $m_{PS} r_0$ is needed. These values are close to the simulated ones, and so even a linear interpolation is usually sufficient. By using the value of the force parameter $r_0 = 0.5 \text{ fm}$ [36, 37], to set the scale, the lowest pseudoscalar meson mass that can be reached corresponds to $m_{PS} = 272 \text{ MeV}$ (for which we have only data obtained with the PCAC definition of $\kappa_c$). On the basis of the study performed in ref. [2], we expect finite size effects (FSE) in the matrix element to be relevant for the smallest four quark masses simulated. Extending the study of ref. [2] down to values of $m_{PS} L \simeq 2.7$ (for which the FSE can be as large as 13%), we have corrected the matrix elements for these effects down to the second smallest
Table 1: Simulation parameters and the number of measurements ($N_{\text{meas}}$)

| $\beta$ | 5.85 | 6.00 | 6.10 | 6.20 | 6.45 |
|--------|------|------|------|------|------|
| $a$ (fm) | 0.123 | 0.093 | 0.079 | 0.068 | 0.048 |
| $r_0/a$ | 4.067 | 5.368 | 6.324 | 7.360 | 10.458 |
| $L/a$ | 16 | 16 | 20 | 24 | 32 |
| $T/a$ | 32 | 32 | 40 | 48 | 64 |

| $N_{\text{meas}}$ | 255 | 388 | 300 | 207 | 214 |
|-----------------|-----|-----|-----|-----|-----|
| $\mu_2a$ | 0.0100 | 0.0076 | 0.0064 | 0.0055 | 0.0039 |
| $\mu_3a$ | 0.0200 | 0.0151 | 0.0128 | 0.0111 | 0.0111 |
| $\mu_4a$ | 0.0400 | 0.0302 | 0.0257 | 0.0221 | 0.0221 |
| $\mu_5a$ | 0.0600 | 0.0454 | 0.0385 | 0.0332 | 0.0332 |
| $\mu_6a$ | 0.0800 | 0.0605 | 0.0514 | 0.0442 | 0.0442 |
| $\mu_7a$ | 0.1000 | 0.0756 | 0.0642 | 0.0553 | 0.0553 |

| $N_{\text{meas}}$ | 400 | 300 | 300 |
|-----------------|-----|-----|-----|
| $\mu_1a$ | 0.0050 | 0.0038 | 0.0028 |
| $\mu_2a$ | 0.0100 | 0.0076 | 0.0055 |
| $\mu_3a$ | 0.0200 | 0.0151 | 0.0111 |
| $\mu_4a$ | 0.0400 | 0.0302 | 0.0221 |
| $\mu_5a$ | 0.0600 | 0.0454 | 0.0332 |
| $\mu_6a$ | 0.0800 | 0.0605 | 0.0442 |
| $\mu_7a$ | 0.1000 | 0.0756 | 0.0553 |

quark mass ($m_{PS}=368$ MeV). For the smallest quark mass, however, the sensitivity required to investigate FSE is computationally very expensive and here we present the corresponding points without corrections, with the purpose of showing that, even for quantities more complicated to extract than meson masses or decay constants, there are no problems of principle in reaching small quark masses.

In fig. 2 we show the combined continuum extrapolation of $\langle x \rangle$ obtained with the two definitions of $\kappa_c$, already converted to the $\overline{\text{MS}}$ scheme at $\mu = 2$ GeV as explained in the previous section, for a wide range of values of fixed pseudoscalar meson masses. In principle, employing the renormalization factors obtained with (untwisted) Wilson fermions O($a$) lattice artifacts can be introduced, which are absent in the bare matrix elements. However this kind of O($a$) effects are independent of the mass and of the definition of the $\kappa_c$ used. Considering for example the case of the second lowest mass $\mu_2$ ($m_{PS} = 368$ GeV) in fig. 2 and performing a combined continuum fit of the type $A + Ba/r_0 + C(a/r_0)^2$ where $A$ and $B$ are the same for the two definitions of $\kappa_c$ while $C$ is different, one finds that $B \approx 0$. Since $B/A$ does not depend upon the mass it follows that in the determination of the renormalization
Table 2: Pseudoscalar meson masses $m_{PSa}$ for all simulation points. These data refer to a subset of the data obtained in ref. \cite{12}.

Factors $O(a)$ lattice artifacts are in practice negligible. We are thus justified in performing a continuum extrapolation of the type $A + C(a/r_0)^2$ and we can see from fig. 2 that the scaling of $\langle x \rangle$ is in agreement with pure $O(a^2)$ cut-off effects for both definitions of the critical mass and values of $\beta \geq 6.0$. The slope of $\langle x \rangle$ as a function of $a^2$ appears to be rather small for the PCAC definition of $\kappa_c$. At $\beta = 5.85$ and lower, lattice artifacts which increase with $\mu$ are visible for the highest masses while, in analogy to what observed in ref. \cite{12}, by using the pion definition of $\kappa_c$ $O(a^2)$ cut-off effects are enhanced at small quark mass. Indeed, for the second smallest pseudoscalar meson mass (the smallest one is absent with the pion definition of $\kappa_c$), we performed an additional simulation at $\beta = 6.45$, in order to have a better control on the continuum extrapolation, and we excluded the point at $\beta = 6.0$ (which appears to be outside of the scaling region). Fig. 2 nicely demonstrates that using only this definition of the critical mass it is important to add the data point at $\beta = 6.45$ and this effect would be probably even worse at the smallest pseudoscalar meson mass.

In fig. 3 and table 4 we present the results for $\langle x \rangle_{MS}^{\mu = 2 GeV}$ in the continuum as a function of the pseudoscalar meson mass in GeV. The empty squares are our values obtained earlier from a combined continuum extrapolation of Wilson and clover-improved Wilson fermions data using the Schrödinger functional scheme \cite{11}. As usual, such quenched simulations have to stop at a pseudoscalar meson mass of about 600 MeV. At such high masses it becomes very difficult, if not impossible, to
Table 3: Renormalization factor $Z^{\text{MS}} \equiv Z_{\text{RGI}}(a)/f_{\text{MS}}^\mu$ for $\mu = 2$ GeV from ref. [1] and bare matrix element $\langle x \rangle^{\text{bare}}$ for all simulation points.

| $\beta$ | 5.85 | 6.00 | 6.10 | 6.20 | 6.45 |
|---------|------|------|------|------|------|
| $Z^{\text{MS}}$ | 0.90(5) | 0.95(4) | 0.99(4) | 1.01(4) | 1.06(5) |

\[
\langle x \rangle^{\text{bare, SF}} (\kappa_c^{\text{pion}})
\]

| $\mu_{2a}$ | 0.2848(105) | 0.2143(107) | 0.2028(93) | 0.2073(103) | 0.2226(108) |
| $\mu_{3a}$ | 0.3295(57) | 0.2818(56) | 0.2700(53) | 0.2621(49) | 0.2996(33) |
| $\mu_{4a}$ | 0.3643(37) | 0.3294(33) | 0.3144(28) | 0.2996(33) | 0.3215(26) |
| $\mu_{5a}$ | 0.3840(25) | 0.3533(24) | 0.3374(21) | 0.3386(24) | 0.3215(26) |
| $\mu_{6a}$ | 0.4012(20) | 0.3711(20) | 0.3551(17) | 0.3386(24) | 0.3215(26) |
| $\mu_{7a}$ | 0.4168(18) | 0.3861(17) | 0.3700(15) | 0.3539(20) | 0.3215(26) |

\[
\langle x \rangle^{\text{bare}} (\kappa_c^{\text{PCAC}})
\]

| $\mu_{1a}$ | 0.2566(157) | 0.2615(219) | 0.2505(241) |
| $\mu_{2a}$ | 0.3049(80) | 0.2819(110) | 0.2698(98) |
| $\mu_{3a}$ | 0.3420(39) | 0.3135(58) | 0.2907(46) |
| $\mu_{4a}$ | 0.3704(24) | 0.3439(36) | 0.3127(31) |
| $\mu_{5a}$ | 0.3900(18) | 0.3631(26) | 0.3300(24) |
| $\mu_{6a}$ | 0.4077(15) | 0.3791(21) | 0.3455(19) |
| $\mu_{7a}$ | 0.4237(13) | 0.3935(18) | 0.3502(16) |

**Table 4:** $\langle x \rangle^{\text{MS}}$ in the continuum using a combined extrapolation of data obtained with the PCAC and pion definition of $\kappa_c$.* The value corresponding to a pseudoscalar meson mass of 272 MeV has not been corrected for FSE.

| $m_{\text{PS}}$ [GeV] | $\langle x \rangle^{\text{MS}}$ |
|----------------------|-------------|
| 0.272*               | 0.260(31)*  |
| 0.368                | 0.243(21)   |
| 0.514                | 0.272(21)   |
| 0.728                | 0.299(22)   |
| 0.900                | 0.317(23)   |
| 1.051                | 0.335(24)   |
| 1.163                | 0.350(25)   |

compare the simulation results to chiral perturbation theory [38, 39, 40] or to other phenomenological predictions [41, 42], even when the results are extrapolated to the continuum limit as done here.

Fig. 3 shows that with Wilson twisted mass fermions, the large gap between pseudoscalar meson masses of about 600 MeV, as the lower bound for standard simulations, and the physical value can be bridged. Quenched chiral perturbation
theory predicts the absence of chiral logs for the matrix element studied in this letter, but our present large error bars, and the lack of more data in the region \((m_{\text{PS}} \lesssim 500 \text{ MeV})\) where chiral perturbation theory should be applicable, does not allow us to perform a careful chiral extrapolation. We quote then as our final result

\[
\langle x \rangle_{\text{MS}}(2\text{GeV}) = 0.243(21)
\] (14)
given by the value at the next to smallest pion mass.

4 Conclusions

In this letter we performed a test of Wilson twisted mass fermions for interesting physical observables, the moments of parton distribution function which are relevant in deep inelastic scattering. So far, most investigations of Wilson twisted mass QCD at small masses considered only 2-point correlation functions. The present study is the first that investigates 3-point correlators down to masses of order 250 MeV. In particular, here we have studied the example of a twist-2 operator. The matrix element of such a renormalized operator between pion states \(\langle x \rangle\) corresponds to the average momentum of the valence quark distribution (up for example) in a pion.

In the present work we employed two definitions of the critical mass, the pion and PCAC definition \([11, 12]\). The scaling of \(\langle x \rangle\) is in agreement with the expected \(O(a^2)\) cut-off effects for both definitions of the critical mass. We could perform a controlled continuum extrapolation of \(\langle x \rangle\) down to pseudoscalar meson masses of about 270 MeV by combining the data obtained with the two definitions. Of course, in principle, also overlap simulations are able to reach such values of the pseudoscalar meson mass. This will come, however, at a much higher simulation cost \([17]\). Our final figure, fig. 3 clearly demonstrates that with our present setup it is possible to bridge the gap between large pseudoscalar meson mass values of 600 MeV and the physical value of the pion mass.

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Figure 2: $\langle x \rangle^{\text{MS}}$ as a function of $(a/r_0)^2$ for different values of the pseudoscalar meson mass.
Figure 3: $\langle x \rangle^{\overline{MS}}(\mu = 2 \text{ GeV})$ extrapolated to the continuum as a function of the pseudoscalar meson mass. Squares are obtained from a combined continuum extrapolation of earlier Wilson and clover improved Wilson simulations \cite{1}. The circles represent our results using Wilson twisted mass fermions. For the empty circle at the smallest mass see the text. The diamond represents the experimental value as obtained from global fits \cite{44, 45}. Recently a new analysis \cite{46} has been performed giving as a result $\langle x \rangle^{\overline{MS}}(\mu = 2.28 \text{ GeV}) = 0.217(11)$. $^a$

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