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Scaling and χPT Description of Pions from $N_{\rm f} = 2$ twisted mass QCD

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We study light-quark observables by means of dynamical lattice QCD simulations using two flavours of twisted mass fermions at maximal twist. We employ chiral perturbation theory to describe our data for the pion mass and decay constant. In this way, we extract precise determinations for the low-energy constants of the effective theory as well as for the light-quark mass and the chiral condensate.

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1. Introduction

In recent years, the non-perturbative description of QCD on the lattice has made a significant breakthrough in tackling the systematic effects present in the determination of several important physical quantities, opening the way for a direct connection to experiments (see *e.g.* [1, 2] for recent reviews). Simulations containing the dynamics of the light-quark flavours in the sea, as well as those due to the strange quark and recently also to the charm, using pseudoscalar masses below 300 MeV, lattice extents $L \geq 2$ fm and lattice spacings smaller than 0.1 fm are presently being performed by several lattice groups. Such simulations will eventually allow for an extrapolation of the lattice data to the continuum limit and to the physical point while keeping also the finite volume effects under control.

The European Twisted Mass collaboration (ETMC) has carried out large scale simulations with $N_f = 2$ flavours of mass degenerate quarks using Wilson twisted mass fermions at maximal twist. Four values of the lattice spacing ranging from 0.1 fm down to 0.051 fm, pseudoscalar masses between 280 and 650 MeV as well as several lattice sizes ($2.0 - 2.5$ fm) are used to address the systematic effects.

The physics of the light pseudoscalar meson is in a suitable sector for investigating the systematic effects arising from the continuum, infinite volume and chiral extrapolations of lattice data, since the pion mass and decay constant can be measured with high statistical accuracy in lattice simulations. Moreover, chiral perturbation theory (χPT) is best understood for those two quantities. As a result of this study one can extract several important quantities, such as the u,d quark masses, the chiral condensate or the low-energy constants of χPT. First results for the pseudoscalar mass $m_{\rm PS}$ and decay constant $f_{\rm PS}$ from these $N_f = 2$ simulations have been presented in Refs. [3–9].

ETMC is currently generating $N_f = 2+1+1$ ensembles including in the sea, in addition to the mass degenerate light u,d quark flavours, also the heavier strange and charm degrees of freedom. First results for the pseudoscalar mass and decay constant from this novel setup were presented in [10, 11].

In the following we will mainly focus on the results from the $N_f = 2$ data for $m_{\rm PS}$ and $f_{\rm PS}$.

2. Lattice Action and Simulation Setup

In the gauge sector we employ the tree-level Symanzik improved gauge action (tlSym) [12]. The fermionic action for two flavours of maximally twisted, mass degenerate quarks [13, 14] in the so-called twisted basis (where the quark field doublets are denoted by χ and $\bar{\chi}$) reads

$$S_{\rm tm} \;=\; a^4 \sum_x \left\{ \bar{\chi}(x) \left[D[U] + m_0 + i\mu_q \gamma_5 \tau^3 \right] \chi(x) \right\} , \tag{2.1}$$

where m_0 is the untwisted bare quark mass tuned to its critical value $m_{\rm crit}$, μ_q is the bare twisted quark mass, τ^3 is the third Pauli matrix acting in flavour space and $D[U]$ is the Wilson-Dirac operator.

At maximal twist, i.e. $m_0 = m_{\rm crit}$, physical observables are automatically O(a) improved without the need to determine any action or operator specific improvement coefficients [14] (for a

Ensemble	β	a [fm]	V/a^4	$m_{PS}L$	$a\mu_q$	m_{PS} [MeV]
D_1	4.20	0.051	$48^3 \cdot 96$	3.6	0.0020	280
D_2			$32^3 \cdot 64$	4.2	0.0065	510
C_1	4.05	0.063	$32^3 \cdot 64$	3.3	0.0030	320
C_2				4.6	0.0060	450
C_3				5.3	0.0080	520
C_4				6.5	0.0120	630
C_5			$24^3 \cdot 48$	3.5	0.0060	450
C_6			$20^3 \cdot 48$	3.0	0.0060	450
B_1	3.90	0.079	$24^3 \cdot 48$	3.3	0.0040	330
B_2				4.0	0.0064	420
B_3				4.7	0.0085	480
B_4				5.0	0.0100	520
B_5				6.2	0.0150	640
B_6			$32^3 \cdot 64$	4.3	0.0040	330
B_7				3.7	0.0030	290
A_2	3.80	0.100	$24^3 \cdot 48$	5.0	0.0080	410
A_3				5.8	0.0110	480
A_4				7.1	0.0165	580

Table 1: Ensembles with $N_f = 2$ dynamical flavours produced by the ETM collaboration. We give the ensemble name, the values of the inverse bare coupling $\beta = 6/g_0^2$, an approximate value of the lattice spacing a, the lattice volume $V = L^3 \cdot T$ in lattice units, the approximate value of $m_{PS}L$, the bare quark mass μ_q in lattice units and an approximate value of the light pseudoscalar mass m_{PS}.

review see Ref. [15]). With this being the main advantage [1], one drawback of maximally twisted mass fermions is that parity and flavour symmetry are broken explicitly at finite values of the lattice spacing, which amounts to $O(a^2)$ effects in physical observables.

For details on the setup, tuning to maximal twist and the analysis methods we refer to Refs. [3, 4, 6]. Recent results for light quark masses, meson decay constants, the pion form factor, π-π scattering, the light baryon spectrum, the η' meson and the $\omega - \rho$ mesons mass difference are available in Refs. [16 – 22].

Flavour breaking effects have been investigated for several quantities [3, 4, 6, 7, 19]. With the exception of the splitting between the charged and neutral pion masses, other possible splittings in the unitary observables so far investigated are found to be compatible with zero. These results are in agreement with a theoretical investigation using the Symanzik effective Lagrangian [23, 24].

A list of the $N_f = 2$ ensembles generated by ETMC can be found in table 1.

3. Scaling to the Continuum Limit

Here we analyse the scaling to the continuum limit of the pseudoscalar meson decay constant

[1] Other properties being, *e.g.*, that the quark mass renormalises only multiplicatively and that the determination of the pseudoscalar decay constant does not require a renormalisation factor.

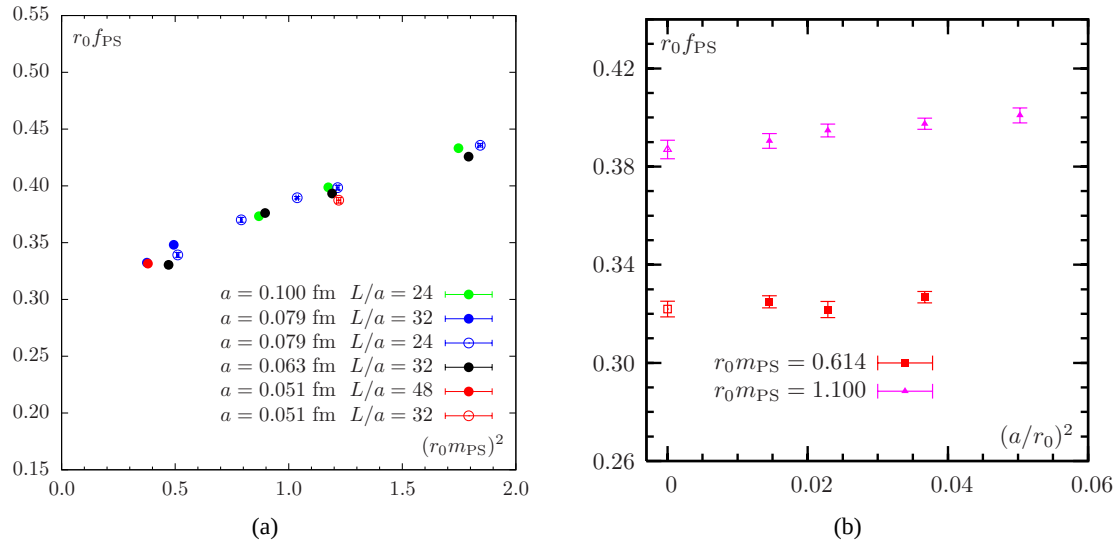

Figure 1: (a) $r_0 f_{PS}$ as a function of $(r_0 m_{PS})^2$. (b) Continuum limit scaling: $r_0 f_{PS}$ as a function of $(a/r_0)^2$ at two fixed values of $r_0 m_{PS}$ and at fixed volume.

f_{PS} at fixed reference values of the pseudoscalar meson mass m_{PS} and of the lattice size L (we refer to [4, 5, 9] for details). The purpose of this scaling test is to verify that discretisation effects are indeed of $O(a^2)$ as expected for twisted mass fermions at maximal twist.

In order to compare results coming from different values of the lattice spacing it is convenient to measure on the lattice the hadronic scale r_0 [25]. It is defined via the force between static quarks at intermediate distance and can be measured to high accuracy in lattice QCD simulations. For details on how we measure r_0/a and on how its chiral extrapolation is performed, we refer to Ref. [6, 9].

In figure 1(a) we plot the raw data for $r_0 f_{PS}$ as a function of $(r_0 m_{PS})^2$. The vicinity of points coming from different lattice spacings along a common curve is an evidence that lattice artifacts are small for these quantities. This is indeed confirmed in figure 1(b) where the continuum scaling of $r_0 f_{PS}$ is illustrated: the very mild slope of the lattice data shows that the expected $O(a^2)$ scaling violations are small. The result of a linear extrapolation in $(a/r_0)^2$ to the continuum limit is also shown.

Analogous continuum limit scaling studies have been performed for the charged pion mass [5, 9] and the nucleon mass [19, 26], showing also in these cases signs of only small scaling violations.

4. χPT Description of Lattice Data

The chiral extrapolation of lattice data down to the physical point is currently one of the main sources of systematic uncertainties in the lattice results. The possibility to rely on an effective theory such as χPT to guide this extrapolation is therefore of great importance to quote accurate results from lattice simulations. On the other hand, while smaller quark masses are becoming accessible in numerical simulations, the possibility to perform a quantitative test of the effective theory as well as to determine the low energy parameters of its Lagrangian becomes more and more realistic.

We now proceed by presenting the results of a combined continuum, chiral and infinite volume extrapolation of $m_{\rm PS}$ and $f_{\rm PS}$ for two values of the lattice spacing (corresponding to $a \approx 0.063$ fm and $a \approx 0.079$ fm). We use the chirally extrapolated values of r_0/a to relate data from the two lattice spacings and a non-perturbative determination of the renormalisation factor $Z_{\rm P}$ [28] in order to perform the fit in terms of renormalised quark masses. This analysis closely follows those presented in Refs. [4, 5, 7–9] to which we refer for more details.

We perform combined fits to our data for $f_{\rm PS}$, $m_{\rm PS}$, r_0/a and $Z_{\rm P}$ at the two values of the lattice spacing with the formulae:

$$\begin{aligned} r_0 f_{\rm PS} &= r_0 f_0 \Big[1 - 2\xi \log\left(\frac{\chi_\mu}{\Lambda_4^2}\right) + T_f^{\rm NNLO} + D_{f_{\rm PS}} (a/r_0)^2\Big] \; K_f^{\rm CDH}(L)\,, \\ (r_0 m_{\rm PS})^2 &= \chi_\mu r_0^2 \Big[1 + \xi \log\left(\frac{\chi_\mu}{\Lambda_3^2}\right) + T_m^{\rm NNLO} + D_{m_{\rm PS}} (a/r_0)^2\Big] \; K_m^{\rm CDH}(L)^2\,, \end{aligned} \tag{4.1}$$

with $\xi \equiv 2B_0\mu_R/(4\pi f_0)^2$, $\chi_\mu \equiv 2B_0\mu_R$, $\mu_R \equiv \mu_q/Z_{\rm P}$, $f_0 \equiv \sqrt{2}F_0$. $T_{m,f}^{\rm NNLO}$ denote the continuum NNLO terms of the chiral expansion [29], which depend on Λ_{1-4} and k_M and k_F. The finite size corrections factors $K_{m,f}^{\rm CDH}(L)$ refer to a continuum χPT description using the resummed Lüscher formula, that we denote as CDH [30]. [2]

Based on the form of the Symanzik expansion in the small quark mass region, we parametrise in eq. (4.1) the leading cut-off effects by the two coefficients $D_{f_{\rm PS},m_{\rm PS}}$. Setting $D_{f_{\rm PS},m_{\rm PS}} = 0$ is equivalent to perform a constant continuum extrapolation. Similarly, setting $T_{m,f}^{\rm NNLO} = 0$ corresponds to fit to NLO χPT.

From the fit parameters related to the quark mass dependence predicted by χPT (in particular from $\Lambda_{3,4}$, B_0 and f_0) the low energy constants $\bar{\ell}_{3,4}$ and the chiral condensate Σ can be determined, using the following expressions:

$$\begin{aligned} \bar{\ell}_i &= \log\left(\frac{\Lambda_i^2}{(m_\pi^\pm)^2}\right)\,, \\ \Sigma &= -\frac{B_0 f_0^2}{2}\,. \end{aligned} \tag{4.2}$$

By including or excluding data points for the heavier quark masses, it is in principle possible to explore the regime of masses in which NLO and/or NNLO SU(2) χPT applies. We have actually generalised this procedure in order to estimate all the dominant sources of systematic uncertainties that can be addressed from our setup, which include, discretisation effects, the order at which we work in χPT or finite size effects. The idea is to use different fit ansätze (see below) on a given data-set and to repeat this same procedure over different data-sets: by weighting all these fits by their confidence level we construct their distribution and estimate the systematic error from the associated 68% confidence interval.

The fit ansätze we consider are:

- Fit A: NLO continuum χPT, $T_{m,f}^{\rm NNLO} \equiv 0$, $D_{m_{\rm PS},f_{\rm PS}} \equiv 0$, priors for $r_0\Lambda_{1,2}$
- Fit B: NLO continuum χPT, $T_{m,f}^{\rm NNLO} \equiv 0$, $D_{m_{\rm PS},f_{\rm PS}}$ fitted, priors for $r_0\Lambda_{1,2}$

[2] For a more detailed description of finite size effects in our data for $m_{\rm PS}$ and $f_{\rm PS}$, we refer to Refs. [4, 9].

$m_{u,d}$ [MeV]	3.54(26)
$\bar{\ell}_3$	3.50(31)
$\bar{\ell}_4$	4.66(33)
f_0 [MeV]	121.5(1.1)
f_π/f_0	1.0755(94)
B_0 [MeV]	2638(200)
$\lvert\Sigma\rvert^{1/3}$ [MeV]	270(7)

Table 2: Summary of fit results. The errors are statistical and systematical, added in quadrature. B_0, Σ and $m_{u,d}$ are (non-perturbatively) renormalised in the $\overline{\rm MS}$ scheme at the scale $\mu = 2$ GeV.

- Fit C: NNLO continuum χPT, $D_{m_{\rm PS},f_{\rm PS}} \equiv 0$, priors for $r_0\Lambda_{1,2}$ and $k_{M,F}$
- Fit D: NNLO continuum χPT, $D_{m_{\rm PS},f_{\rm PS}}$ fitted, priors for $r_0\Lambda_{1,2}$ and $k_{M,F}$

The choice of the different data-sets (each of them including data for different lattice spacings, quark masses and physical volumes) is made in order to quantify how the quality of the fit is modified when including/excluding data from *e.g.*, a given mass region or with a given volume. The data-sets considered in the fits are listed in Ref. [9].

The parameters $k_{M,F}$ and $r_0\Lambda_{1,2}$ appearing at NNLO (and in the latter case, also at higher order in the CDH expressions) need to be fitted with some additional input information (priors). Additional lattice data would be needed to allow these parameters to remain free in the fit. The parameters $r_0\Lambda_{1,2}$ use priors from the estimates for $\bar{\ell}_{1,2}$ in Ref. [30], while very mild priors are used for $k_{M,F} = 0 \pm 10$. For a detailed description of the use of priors and, in general, of the statistical analysis, we refer to Ref. [9].

The results of the combined fits to data from the two lattice spacings $a \approx 0.063$ fm and $a \approx 0.079$ fm are given in table 2. The errors are statistical and systematical, added in quadrature. For a review on the determination of the low-energy constants and of the light-quark mass we refer to [31, 32, 2]. Recent determinations from ETMC of the pseudoscalar decay constant and chiral condensate in the ε-regime were presented in [33].

As a further check, we have performed additional fits including either the finer lattice spacing ($a \approx 0.051$ fm) or the coarser one ($a \approx 0.100$ fm) finding total compatibility with the results of table 2.

5. Discussion and Conclusion

Here we collect a short list of observations coming from a set of χPT fits. A complete description of these fits was presented in Ref. [9].

We observe that including in the fits pseudoscalar masses $m_{\rm PS} > 520$ MeV decreases significantly the quality of the NLO fits ($\chi^2/{\rm dof} \gg 1$). This indicates that the applicability of NLO χPT in that regime of masses is disfavoured.

On the contrary, extending the fit-range to a value of $m_{\rm PS} \sim 280$ MeV preserves the good quality of the fit and gives compatible values for the fit parameters. This result makes us confident that the extrapolation to the physical point is trustworthy.

Including lattice artifacts in the fits gives results which are compatible to those where $D_{m_{PS},f_{PS}}$ is set to zero but with a somehow better χ^2/dof. We observe that the values of the fitting parameters $D_{m_{PS},f_{PS}}$ are compatible with zero within two standard deviations. This is in line with the small discretisation effects observed in the scaling test.

The inclusion of NNLO terms produces similar results to the NLO fits in the quark mass region corresponding to $m_{PS} \in [280, 520]$ MeV. When fitting data only in this mass region (*i.e.* when excluding from the fit the heavier masses at $m_{PS} \sim 650$ MeV), we observe that the fit curve at NLO lies closer to those data points (heavier masses) than the NNLO one. On the other hand, when including the heavier masses, the NNLO fit is able describe these data points but the quality of the fit is somehow reduced with respect to the NLO fit. To improve the sensitivity of our lattice data to χPT at NNLO, additional data points would be needed.

We have presented determinations of f_{PS} and m_{PS} and of their continuum, infinite volume and chiral extrapolations. As a result, we obtain accurate determinations of the u, d quark mass, the chiral condensate as well as of low-energy constants of the effective theory, including an exhaustive estimate for the systematic uncertainties.

The only systematic effect which cannot be addressed by this study corresponds to effect of the strange and the charm quarks in the sea. We are currently in the process of extending this analysis to the $N_f = 2+1+1$ ensembles which are being generated by ETMC [10, 11].

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