PROCEEDINGS OF SCIENCE

DESY 09-063, SFB/CPP-09-38

χPT description of the pion mass and decay constant from $N_f = 2$ twisted mass QCD

Petros Dimopoulos, Roberto Frezzotti
Dipartimento di Fisica, Università di Roma "Tor Vergata"
Via della Ricerca Scientifica 1, 00133 Rome, Italy
E-mail: `{dimopoulos,frezzotti}@roma2.infn.it`

Gregorio Herdoiza*, **Karl Jansen**
DESY
Platanenallee 6, 15738 Zeuthen, Germany
E-mail: `{Gregorio.Herdoiza,Karl.Jansen}@desy.de`

Chris Michael
Theoretical Physics Division, Department of Mathematical Sciences, University of Liverpool
Liverpool L69 3BX, UK
E-mail: `c.michael@liverpool.ac.uk`

Carsten Urbach
Humboldt-Universität zu Berlin, Institut für Physik,
Newtonstr. 15, 12489 Berlin, Germany
E-mail: `Carsten.Urbach@physik.hu-berlin.de`

for the ETM Collaboration

We study lattice QCD determinations of the pion mass and decay constant by means of chiral perturbation theory (χPT). The lattice data are obtained from large scale simulations with $N_f = 2$ flavours of twisted mass fermions at maximal twist. We perform a scaling test to the continuum limit of these data and use χPT to perform both the chiral and the infinite volume extrapolations.

International Workshop on Effective Field Theories: from the pion to the upsilon
February 2-6 2009
Valencia, Spain

*Speaker.

PoS(EFT09)039

1. Introduction

In the last few years, lattice QCD simulations have made a substantial progress in controlling the systematic effects present in the determination of several important physical quantities allowing therefore for their direct contact with experiment (see [1] for a recent review). Simulations including the light-quark flavours in the sea, as well as the strange and recently also the charm, with pseudoscalar masses below 300 MeV, lattice extents $L > 2.5$ fm and lattice spacings smaller than 0.1 fm are currently being performed by several lattice groups. Such simulations will eventually allow for an extrapolation of the lattice data to the physical point and to the continuum limit while keeping also the finite volume effects under control.

The European Twisted Mass collaboration (ETMC) has performed large scale simulations with $N_\mathrm{f} = 2$ 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 0.055 fm, pseudoscalar masses between 270 and 600 MeV as well as several lattice sizes $(2.1-2.8$ fm) are used to address the systematic effects.

The light pseudoscalar meson is in an appropriate hadron for investigating the systematic effects arising from continuum, thermodynamic and chiral extrapolations, because its mass and decay constant can be obtained with high statistical precision in lattice simulations. Moreover, chiral perturbation theory (χPT) is best understood for those two quantities. As a consequence of this study one can extract other quantities of phenomenological interest, such as the u,d quark masses, the chiral condensate or the low energy constants of χPT. First results for the pseudoscalar mass m_PS and decay constant f_PS from these $N_\mathrm{f} = 2$ simulations can be found in Refs. [2 – 6].

ETMC is currently performing $N_\mathrm{f} = 2+1+1$ simulations including in the sea, in addition to the mass degenerate light u,d quark flavours, also the heavier strange and charm degrees of freedom. Some first results for the pseudoscalar mass and decay constant from this novel setup were presented in [7].

In the following we will concentrate on the analysis of the $N_\mathrm{f} = 2$ data for m_PS and f_PS.

2. Lattice Action and Setup

In the gauge sector we employ the tree-level Symanzik improved gauge action (tlSym) [8]. The fermionic action for two flavours of maximally twisted, mass degenerate quarks in the so-called twisted basis [9, 10] reads

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

where m_0 is the untwisted bare quark mass tuned to its critical value m_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. $m_0 = m_\mathrm{crit}$, physical observables are automatically $\mathrm{O}(a)$ improved without the need to determine any action or operator specific improvement coefficients [10] (for a review see Ref. [11]). With this being the main advantage, one drawback of maximally twisted mass fermions is that flavour symmetry is broken explicitly at finite value of the lattice spacing, which amounts to $\mathrm{O}(a^2)$ effects in physical observables.

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Ensemble	β	a [fm]	V/a^4	$m_{PS}L$	$a\mu_q$	m_{PS} [MeV]
D_1	4.20	0.055	$48^3 \cdot 96$	3.6	0.0020	270
D_2			$32^3 \cdot 64$	4.2	0.0065	480
C_1	4.05	0.065	$32^3 \cdot 64$	3.3	0.0030	310
C_2				4.6	0.0060	430
C_3				5.3	0.0080	500
C_4				6.5	0.0120	610
C_5			$24^3 \cdot 48$	3.5	0.0060	430
C_6			$20^3 \cdot 48$	3.0	0.0060	430
B_1	3.90	0.085	$24^3 \cdot 48$	3.3	0.0040	315
B_2				4.0	0.0064	390
B_3				4.7	0.0085	450
B_4				5.0	0.0100	490
B_5				6.2	0.0150	600
B_6			$32^3 \cdot 64$	4.3	0.0040	310
B_7				3.7	0.0030	270
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 coupling β, 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}.

For details on the setup, tuning to maximal twist and the analysis methods we refer to Refs. [2, 3, 5]. Recent results for light quark masses, meson decay constants, the pion form factor, the light baryon spectrum, the η' meson and the $\omega - \rho$ mesons mass difference are available in Refs. [12 – 17].

Flavour breaking effects have been investigated for several quantities [2, 3, 5, 6, 14]. With the exception of the splitting between the charged and neutral pion masses, other possible splittings so far investigated are compatible with zero. These results are in agreement with a theoretical investigation using the Symanzik effective Lagrangian [18].

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

3. Results

3.1 Scaling to the Continuum Limit

Here we analyse the scaling to the continuum limit of the pseudoscalar meson decay constant f_{PS} at fixed reference values of the pseudoscalar meson mass m_{PS} and of the lattice size L (we refer to [3, 4] for details). The aim 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.

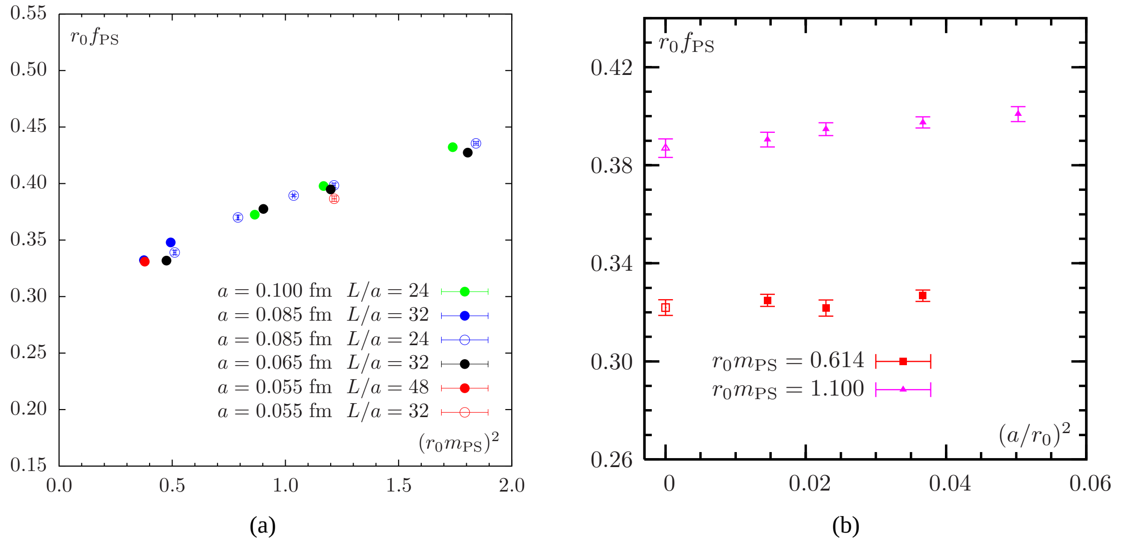

Figure 1: (a) $r_0 f_{PS}$ as a function of $(r_0 m_{PS})^2$ (b) Continuum limit scaling: $r_0 f_{PS}$ as a function of $(a/r_0)^2$ at two fixed values of $r_0 m_{PS}$.

In order to compare results at different values of the lattice spacing it is convenient to measure the hadronic scale r_0/a [19]. 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 we refer to Ref. [5].

In figure 1(a) we plot the results 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.

3.2 χPT Description of Finite Size Effects

At the level of statistical accuracy we have achieved, finite size effects (FSE) for f_{PS} and m_{PS} cannot be neglected. It is therefore of importance to study whether FSE can be described within the framework of chiral perturbation theory. This requires to compare simulations with different lattice volumes while all other parameters are kept fixed, like for instance ensembles C_2, C_5 and C_6 or B_1 and B_6 in table 1. For all these ensembles $m_{PS}L \geq 3$ holds, which is believed to be needed for χPT formulae to apply. Given the smallness of the lattice artifacts in f_{PS} and m_{PS} (as discussed in the previous section), we proceed to compare the *measured* finite size effects to predictions of *continuum* χPT at NLO [20] (denoted GL) and in the form of the resummed Lüscher formula as described in Ref. [23] (for short CDH).

We note $R_O = [O(L=\infty) - O(L)]/O(L=\infty)$ the relative FSE for the observable $O \in \{m_{PS}, f_{PS}\}$. The results for R^{meas}, R^{GL} and R^{CDH} are compiled in table 2. We observe that the CDH formulae tend to provide an appropriate description of the lattice data. A more detailed description of FSE in our f_{PS} and m_{PS} data was presented in Ref. [3].

	a [fm]	$m_{\rm PS}L_1 \to m_{\rm PS}L_2$	$R^{meas.}$[%] $[L_1 \to L_2]$	R^{GL} [%] $[L_1 \to \infty]$	R^{CDH} [%] $[L_1 \to \infty]$
$m_{\rm PS}$	0.085	$3.3 \to 4.3$	-1.8	-0.6	-1.2
$f_{\rm PS}$	0.085	$3.3 \to 4.3$	$+2.6$	$+2.6$	$+2.6$
$m_{\rm PS}$	0.065	$3.0 \to 4.6$	-6.1	-1.9	-6.3
$f_{\rm PS}$	0.065	$3.0 \to 4.6$	$+10.7$	$+7.0$	$+9.0$

Table 2: Comparison of measured relative FSE, R_O, to estimates from χPT formulae.

3.3 χPT Description of the light-quark Mass Dependence

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 perform this extrapolation is therefore of great importance to quote accurate results from lattice simulations. On the other hand, while smaller quark masses are being simulated, the possibility to perform a quantitative test of the effective theory as well as to measure the low energy parameters of its Lagrangian becomes more and more realistic.

We shall now present the results of a combined chiral, thermodynamic and continuum extrapolation of $m_{\rm PS}$ and $f_{\rm PS}$ for two values of the lattice spacing (corresponding to $\beta = 3.9$ and $\beta = 4.05$). We use r_0/a to relate data from the two lattice spacings and a non-perturbative determination of the renormalisation factor $Z_{\rm P}$ [21] in order to perform the fit in terms of renormalised quark masses. This analysis closely follows those presented in Refs. [3, 4, 6] 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 β with the formulae:

$$
\begin{aligned}
r_0 f_{\rm PS} &= r_0 f_0 \left[1 - 2\xi \log\left(\frac{\chi_\mu}{\Lambda_4^2}\right) + T_f^{\rm NNLO} + D_{f_{\rm PS}}(a/r_0)^2\right] K_f^{\rm CDH}(L)\,, \\
(r_0 m_{\rm PS})^2 &= \chi_\mu r_0^2 \left[1 + \xi \log\left(\frac{\chi_\mu}{\Lambda_3^2}\right) + T_m^{\rm NNLO} + D_{m_{\rm PS}}(a/r_0)^2\right] K_m^{\rm CDH}(L)^2\,,
\end{aligned}
\tag{3.1}
$$

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 [22], which depend on Λ_{1-4} and k_M and k_F, and $K_{m,f}^{\rm CDH}(L)$ the finite size corrections [23]. Based on the form of the Symanzik expansion in the small quark mass region, we parametrise in eq. (3.1) 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 coming from 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. Moreover, 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 χPT apply.

As an example, we consider three of such fits:

- Fit A: NLO continuum χPT (*i.e.* $T_{m,f}^{\rm NNLO} \equiv 0$), $D_{m_{\rm PS},f_{\rm PS}} \equiv 0$, ensembles $B_{1,2,3,4,6}$ and $C_{1,2,3,5}$

- Fit B: NLO continuum χPT (*i.e.* $T_{m,f}^{\rm NNLO} \equiv 0$), $D_{m_{\rm PS},f_{\rm PS}}$ fitted, ensembles $B_{1,2,3,4,6}$ and $C_{1,2,3,5}$

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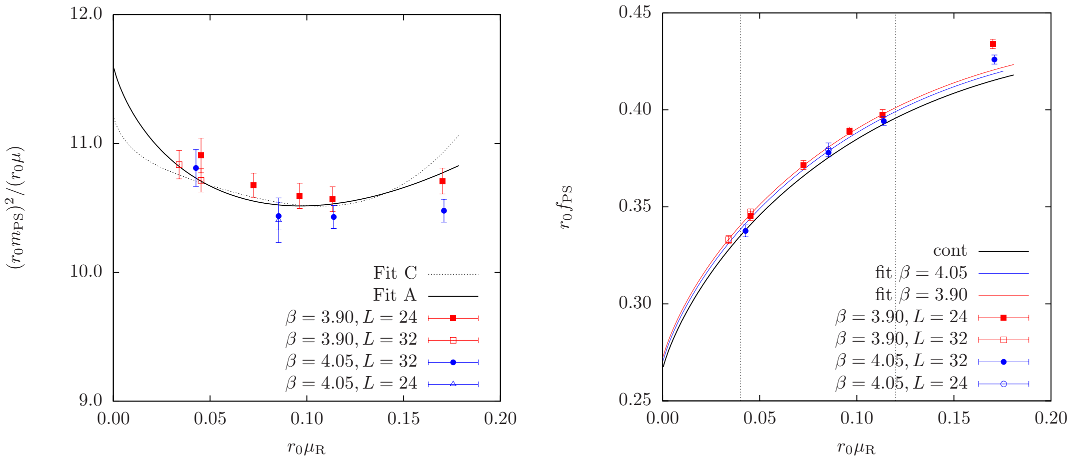

(a) (b)

Figure 2: Quark mass dependence: (a) Data for $(r_0 m_{PS})^2/r_0\mu_R$ as a function of $r_0\mu_R$ and Fits A and C. (b) Data for $r_0 f_{PS}$ as a function of $r_0\mu_R$ and resulting curves of Fit B. The vertical lines indicate the fit range.

- Fit C: NNLO continuum χPT, $D_{m_{PS},f_{PS}} \equiv 0$, ensembles $B_{1,2,3,4,6}$ and $C_{1,2,3,5}$

The quarks mass dependence of $(r_0 m_{PS})^2/r_0\mu_R$ (together with Fits A and C) and of $r_0 f_{PS}$ (with Fit B) are illustrated in figures 2(a) and 2(b).

3.4 Discussion and Conclusion

Here we collect a short list of observations coming from a set of χPT fits. A complete description of these fits will be presented in Ref. [24].

We observe that including in the fits pseudoscalar masses $m_{PS} > 500$ MeV decreases significantly the quality of the NLO fits ($\chi^2/\text{dof} \gg 1$). 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 $m_{PS} \sim 270$ 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. Indeed, when fitting the $D_{m_{PS},f_{PS}}$ parameters we observe that their values are compatible with zero within errors. 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 $0.04 \leq r_0\mu_R \leq 0.12$. When fitting data only in this mass region (*i.e.* when excluding from the fit the heavier masses at $r_0\mu_R \sim 0.17$), 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.

We have presented determinations of f_{PS} and m_{PS} and their continuum, thermodynamic and chiral extrapolations. A complete description of these fits, including the determination of the u,d quark mass, the chiral condensate as well as of low-energy constants of the effective theory will be presented in Ref. [24].

We thank all members of ETMC for the most enjoyable collaboration.

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