SU(2) chiral fits to light pseudoscalar masses and decay constants

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We present the results of fits to recent asqtad data in the light pseudoscalar sector using SU(2) partially-quenched staggered chiral perturbation theory. Superfine ($a \approx 0.06$ fm) and ultrafine ($a \approx 0.045$ fm) ensembles are used, where light sea quark masses and taste splittings are small compared to the strange quark mass. Our fits include continuum NNLO chiral logarithms and analytic terms. We give preliminary results for the pion decay constant, SU(2) low-energy constants and the chiral condensate in the two-flavor chiral limit.

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1. Introduction

At present, most lattice QCD simulations are performed at unphysical light dynamical quark masses. Fitting of lattice data to forms calculated in chiral perturbation theory (χPT) [1, 2] makes possible a controlled extrapolation of lattice results to the physical light quark masses and to the chiral limit. This approach also allows one to determine the values of low-energy constants (LECs) in the theory, which are of phenomenological significance. Although three-flavor χPT has been used successfully for simulations with 2+1 dynamical quarks, we are still interested in the applications of two-flavor χPT for the following reasons:

1. The up and down dynamical quark masses in simulations are usually much smaller than the strange quark mass, which is near its physical value, hence SU(2) χPT may serve as a better approximation and probably converges faster than SU(3) χPT.

2. Fits to SU(2) χPT can give us direct information about the LECs in the two-flavor theory, especially l_3 and l_4.

3. By comparing results from these two different fits, we can study the systematic errors resulting from the truncations of each version of χPT.

Recently, some groups have used SU(2) χPT for chiral fits to data from three-flavor simulations [3, 4]. Here, we perform such an SU(2) chiral analysis for MILC data from simulations with 2+1 flavors of staggered fermions.

2. Rooted SU(2) SχPT

For staggered quarks, the correct effective field theory is staggered chiral perturbation theory (SχPT) [5, 6, 7, 8, 9], in which taste-violating effects at finite lattice spacing are incorporated systematically. Physical quantities expressed in SχPT become joint expansions in both the quark mass m_q and a^2, where a is the lattice spacing.

For each quark flavor, there are four species (tastes) in the continuum limit. To obtain physical results, we use the fourth root procedure to get a single taste per flavor in the continuum limit. Although it has been shown that this procedure produces violations of locality at non-zero lattice spacing non-perturbatively [10], recent work indicates that locality and universality are restored in the continuum limit. For a recent review of the fourth-root procedure see Ref. [11] and references therein.

In the two-flavor case, only up and down quarks appear in the chiral theory. Correspondingly, there are only pions, and no kaons, in SU(2) SχPT. The staggered Lagrangian is formulated in the same way as in Ref. [6], except that those parts related to the strange quark are omitted. Following the procedures used in the three-flavor case, one can calculate the partially-quenched light pseudoscalar mass and decay constant through NLO. The result is [12]:

$$
\begin{aligned}
\frac{m_{P_5^+}^2}{(m_x + m_y)} =& \mu\Big\{ 1 + \frac{1}{16\pi^2 f^2}\Big(\sum_j R_j^{[2,1]}(\{\mathcal{M}_{XY_I}^{[2]}\})l(m_j^2) \\
&- 2a^2\delta_V'\sum_j R_j^{[3,1]}(\{\mathcal{M}_{XY_V}^{[3]}\})l(m_j^2) + (V \leftrightarrow A) + a^2(L_{(2)}'' + L_{(2)}')\Big) \\
&+ \frac{\mu}{f^2}(4l_3 + p_1 + 4p_2)(m_u + m_d) + \frac{\mu}{f^2}(-p_1 - 4p_2)(m_x + m_y)\Big\},
\end{aligned}
\tag{2.1}
$$

$$f_{P_5^+} = f\Big\{1 + \frac{1}{16\pi^2 f^2}\Big[-\frac{1}{32}\sum_{Q,B} l(m_{Q_B}^2)$$

$$+ \frac{1}{4}\Big(l(m_{X_I}^2) + l(m_{Y_I}^2) + (m_{U_I}^2 - m_{X_I}^2)\tilde{l}(m_{X_I}^2) + (m_{U_I}^2 - m_{Y_I}^2)\tilde{l}(m_{Y_I}^2)\Big)$$

$$- \frac{1}{2}\Big(R_{X_I}^{[2,1]}(\{\mathscr{M}_{XY_I}^{[2]}\})l(m_{X_I}^2) + R_{Y_I}^{[2,1]}(\{\mathscr{M}_{XY_I}^{[2]}\})l(m_{Y_I}^2)\Big)$$

$$+ \frac{a^2\delta_V'}{2}\Big(R_{X_V}^{[2,1]}(\{\mathscr{M}_{X_V}^{[2]}\})\tilde{l}(m_{X_V}^2) + \sum_j D_{j,X_V}^{[2,1]}(\{\mathscr{M}_{X_V}^{[2]}\})l(m_j^2)$$

$$+ (X \leftrightarrow Y) + 2\sum_j R_j^{[3,1]}(\{\mathscr{M}_{XY_V}^{[3]}\})l(m_j^2)\Big) + (V \leftrightarrow A)$$

$$+ a^2(L_{(2)}'' - L_{(2)}')\Big] + \frac{\mu}{2f^2}(4l_4 - p_1)(m_u + m_d) + \frac{\mu}{2f^2}(p_1)(m_x + m_y)\Big\}. \qquad (2.2)$$

where l_3 and l_4 are the standard SU(2) $\mathcal{X}$PT LECs, and p_1 and p_2 are two extra NLO LECs that enter in the partially-quenched case. δ_V', δ_A' are taste-violating hairpin parameters, and $L_{(2)}'$, $L_{(2)}''$ are taste-violating analytic LECs. Chiral logarithms $l(m^2)$, $\tilde{l}(m^2)$ and residue functions R, D are given in Ref. [6], with the denominator mass-set arguments in the SU(2) case defined as:

$$\{\mathscr{M}_{X_V}^{[2]}\} \equiv \{m_{X_V}, m_{\eta_V'}\}, \qquad\qquad \{\mathscr{M}_{Y_V}^{[2]}\} \equiv \{m_{Y_V}, m_{\eta_V'}\},$$

$$\{\mathscr{M}_{XY_I}^{[2]}\} \equiv \{m_{X_I}, m_{Y_I}\}, \qquad\qquad \{\mathscr{M}_{XY_V}^{[3]}\} \equiv \{m_{X_V}, m_{Y_V}, m_{\eta_V'}\}. \qquad (2.3)$$

The numerator mass-set arguments of the residues are always $\{\mu_\Xi\} \equiv \{m_{U_\Xi}\}$, where the taste label Ξ is taken equal to the taste of the denominator set.

To Eqs. (2.1) and (2.2), we add the NNLO chiral logarithms that were calculated by Bijnens and Lähde [13]. Since taste splittings are not included at NNLO, there is an ambiguity in defining the pion mass in the continuum formulae. In practice, we use the root mean square (RMS) average pion mass in calculations of NNLO chiral logarithms. This is systematic at NNLO as long as the taste splittings between different pions are significantly less than the pion masses themselves. This condition is best satisfied on the superfine and ultrafine lattices.

3. Ensembles and Data Sets

At the present stage, we have the MILC data for the light pseudoscalar mass and decay constant at five lattice spacings from 0.15 fm to 0.045 fm, generated with 2+1 flavors of asqtad improved staggered quarks. For each lattice spacing, we have several different sea quark masses as well as many different combinations of valence quark masses. In order for the SU(2) formulae to apply, we require both sea and valence quark masses to be significantly smaller than the strange quark mass, *i.e.*, $m_\pi^{sea} \ll m_K$, and $m_\pi^{valence} \ll m_K$. In the fits described below, we use the following cutoff on our data sets:

$$m_l \le 0.2 m_s^{phys}, \qquad m_x + m_y \le 0.5 m_s^{phys}, \qquad (3.1)$$

where m_l is the light sea quark mass, and m_x and m_y are the valence masses in the pion.

To be able to consider the strange quark as "heavy" and eliminate it from the chiral theory, it is also necessary that taste splittings between different pion states be much smaller than the kaon

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Ensemble	am_l	am_s	β	size	$m_\pi L$
≈ 0.09 fm (F)	0.0062	0.031	7.09	$28^3 \times 96$	4.14
≈ 0.09 fm (F)	0.00465	0.031	7.085	$32^3 \times 96$	4.10
≈ 0.09 fm (F)	0.0031	0.031	7.08	$40^3 \times 96$	4.22
≈ 0.09 fm (F)	0.00155	0.031	7.075	$64^3 \times 96$	4.80
≈ 0.06 fm (SF)	0.0036	0.018	7.47	$48^3 \times 144$	4.50
≈ 0.06 fm (SF)	0.0025	0.018	7.465	$56^3 \times 144$	4.38
≈ 0.06 fm (SF)	0.0018	0.018	7.46	$64^3 \times 144$	4.27
≈ 0.045 fm (UF)	0.0028	0.014	7.81	$64^3 \times 192$	4.56

Table 1: Ensembles used in this analysis. The quantities am_l and am_s are the light and strange sea quark masses in lattice units; $m_\pi L$ is the (sea) Goldstone pion mass times the linear spatial size. The fine ensembles are not used in our central value fit, but only in estimating systematic errors.

a	≈ 0.09 fm (F)		≈ 0.06 fm (SF)		≈ 0.045 fm (UF)
am_S	0.031		0.018		0.014
am_l	0.00155	0.0062	0.0018	0.0036	0.0028
m_K(MeV)	574	613	525	548	565
$m_\pi^{\text{Goldstone}}$(MeV)	177	355	224	317	324
m_π^{RMS}(MeV)	281	416	258	341	334
m_π^{I}(MeV)	346	463	280	359	341

Table 2: Kaon masses and lightest (sea) pion masses on some sample ensembles. Here three different pion masses are shown: Goldstone, RMS and singlet. $r_1 = 0.3117$ fm is used.

mass. Furthermore, taste splittings should be significantly smaller than the pion mass itself for the continuum formulae for the NNLO chiral logarithms to be approximately applicable.

The lattices that are at least close to satisfying all these conditions include four fine (a ≈ 0.09 fm) ensembles, three superfine (a ≈ 0.06 fm) ensembles and one ultrafine ensemble (a ≈ 0.045 fm). Relevant parameters for these ensembles are listed in Table 1.

In Table 2, we list the Goldstone, RMS and singlet pion masses on representative ensembles. It can be seen that for the fine (a ≈ 0.09 fm) ensembles, either some pion masses are close to the kaon mass, as on ensemble $(am_l, am_s) = (0.0062, 0.031)$, or the taste splittings between pions are comparable to the pion mass, as on ensemble $(am_l, am_s) = (0.00155, 0.031)$. As a result, the data from fine lattices may not be well described by SU(2) formulae with continuum NNLO chiral logarithms. Our central fit uses superfine and ultrafine data only, while we include fits to all three kinds of lattices to estimate systematic errors.

There are a total of 29 parameters in our fits. The following list shows how these parameters are treated in the central fit.

(a) LO: 2 unconstrained parameters, μ and f.

(b) NLO (physical): 4 parameters, l_3, l_4 and two extra LECs p_1, p_2 that only appear in partially-quenched χPT. All of these parameters are unconstrained.

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(c) NLO (taste-violating): 4 parameters. δ_V', δ_A' are constrained within errors at the values determined from SU(3) SχPT fits [14, 15]; $L_{(2)}''$ and $L_{(2)}'$ are constrained around 0, with width of 0.3 as estimated in Ref. [14].

(d) NNLO (physical, $\mathcal{O}(p^4)$): 5 parameters (l_1, l_2, l_7, p_3, p_4) that first appear in meson masses and decay constants in the NNLO chiral logarithms. l_1 and l_2 are constrained by the range determined from continuum phenomenology [16]; l_7 is not constrained since it is not directly known from phenomenology [16]. The partially-quenched parameters p_3 and p_4 are not constrained.

(e) NNLO (physical, $\mathcal{O}(p^6)$): 8 parameters c_i, constrained around 0 with width 1 in "natural units" (see Ref. [14]).

(f) The physical LO and NLO parameters are allowed to vary with lattice spacing by an amount proportional to $\alpha_s(a\Lambda)^2$, which is the size of the "generic" discretization errors with asqtad quarks, where Λ is some typical hadronic scale. This introduces 6 additional parameters that are constrained around 0 with width corresponding to a scale $\Lambda = 0.7\,\text{GeV}$.

Alternative versions of the fits, in which the width of the constraints are changed, or some constrained parameters are left unconstrained (or *vice versa*), have also been tried, and the results from those fits are included in the systematic error estimates.

4. Preliminary Results

For the central fit, we use three superfine ensembles $(am_l, am_s) = \{(0.0018, 0.018), (0.0025, 0.018), (0.0036, 0.018)\}$ and one ultrafine ensemble $(am_l, am_s) = (0.0028, 0.014)$. This fit has a χ^2 of 37 with 33 degrees of freedom, giving a confidence level CL = 0.3. The volume dependence at NLO has been included in the fit formulae. A very small ($\leq 0.3\%$) correction for "residual" finite volume effects [17, 18] is applied at the end of the calculation and incorporated in the systematic errors of our final results.

In Fig. 1, we show the fit results for f_π and $m_\pi^2/(m_x + m_y)$ as functions of the sum of the quark masses $(m_x + m_y)$. The red curves show the complete results through NNLO for full QCD in the continuum, where we have set taste splitting and taste-violating parameters to zero, extrapolated physical parameters as $a \to 0$ linearly in $\alpha_s a^2$, and set valence quark masses and light sea quark masses equal. Continuum results through NLO and at tree level are shown by blue and magenta curves, respectively. It can be seen that the convergence of SU(2) χPT is much better for the decay constant than for the mass. Nevertheless, the chiral corrections in both cases appear to be under control.

The SU(2) plots presented previously in Ref. [19] are somewhat different from those shown here because the earlier fits allowed for a^2 variations in the NNLO analytic parameters (c_i). Such variations are of higher order than the NNLO terms included in this work.

At the last step, we find the physical values of the average u, d quark mass $\hat{m}$ by requiring that the π has its physical mass, and then find the decay constant corresponding to this point in Fig. 1 (left). With the scale parameter $r_1 = 0.318(7)\,\text{fm}$ [14] determined from Υ-splittings, we obtain the result for f_π:

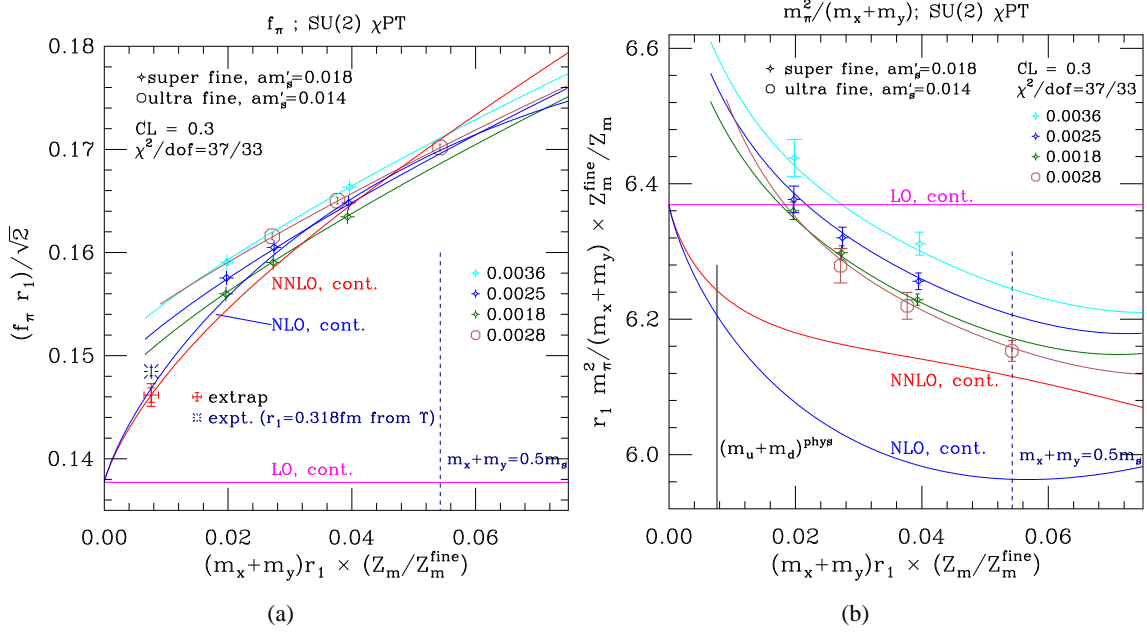$$f_\pi = 128.3(9) \left(^{+20}_{-8}\right) \text{MeV} \tag{4.1}$$

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Figure 1: SU(2) chiral fits to f_π(left) and $m_\pi^2/(m_x + m_y)$(right). Only points with the valence quark masses equal ($m_x = m_y$) are shown on the plots

where the first error is statistical and the second is systematic. This agrees with the PDG 2008 value, $f_\pi = 130.4 \pm 0.2\,\text{MeV}$ [20]. Alternatively, using the pion decay constant from NNLO SU(3) χPT fits to define our scale gives $r_1 = 0.3117(6)\left(^{+12}_{-31}\right)$ fm [15]. With this new r_1, we obtain:

$$
\begin{array}{ll}
f_2 = 123.7(9)(18)\,\text{MeV} & B_2 = 2.89(2)\left(^{+3}_{-8}\right)(14)\,\text{MeV} \\[2mm]
\bar{l}_3 = 3.0(6)\left(^{+9}_{-6}\right) & \bar{l}_4 = 3.9(2)(3) \\[2mm]
\hat{m} = 3.21(3)(5)(16)\,\text{MeV} & \langle \bar{u}u \rangle_2 = -[280(2)\left(^{+4}_{-7}\right)(4)\,\text{MeV}]^3
\end{array}
\tag{4.2}
$$

The quark masses and chiral condensate are evaluated in the $\overline{\text{MS}}$ scheme at $2\,\text{GeV}$. We use the two-loop renormalization factor in the conversion [21]. Errors from perturbative calculations are listed as the third error in these quantities. All the quantities agree with results from SU(3) SχPT fits [15] within errors.

5. Discussion and Outlook

We have performed NNLO SU(2) chiral fits to recent asqtad data in the light pseudoscalar sector. Results for SU(2) LECs, the pion decay constant, and the chiral condensate in the two-flavor chiral limit are in good agreement with those obtained from NNLO SU(3) fits (supplemented by higher-order analytic terms for quantities involving strange valence quarks)[15]. It can be seen from our plots that SU(2) χPT within its applicable region converges much faster than SU(3) χPT. For the point 0.05 on the x-axis in Fig. 1, the ratio of the NNLO correction to the result through NLO is 0.3% for f_π and 2.6% for $m_\pi/(m_x + m_y)$. In contrast, the corresponding numbers in the SU(3) fits are 2.9% and 15.6% respectively (Fig. 2 of Ref. [15]), although the large correction in the mass case is partly the result of an anomalously small NLO term. Note that the SU(3) plots

use a non-physical strange quark mass, $m_s = 0.6 m_s^{phys}$, while for the SU(2) plots, the strange quark mass is near the physical value, $m_s \approx m_s^{phys}$. This explains why the two-flavor chiral limits on the SU(3) and SU(2) plots are not the same.

Since the simulated strange quark masses vary slightly between different ensembles, the parameters in SU(2) SχPT should also change with ensemble [12]. We plan to incorporate this effect in our fit to see if we can improve the confidence levels. Another step would be to include the kaon as a heavy particle in SU(2) SχPT [22] in order to study the physics involving the strange quark, *e.g.*, the kaon mass and decay constant. This approach has recently been used in Refs. [3, 4].

Acknowledgments

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