Staggered chiral perturbation theory in the two-flavor case and SU(2) analysis of the MILC data

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In the light pseudoscalar sector, we study rooted staggered chiral perturbation theory in the two-flavor case. The pion mass and decay constant are calculated through NLO for a partially-quenched theory. In the limit where the strange quark mass is large compared to the light quark masses and the taste splittings, we show that the SU(2) staggered chiral theory emerges from the SU(3) staggered chiral theory, as expected. Explicit relations between SU(2) and SU(3) low energy constants and taste-violating parameters are given. A brief summary of updated SU(2) chiral fits to the MILC lattice data is presented.

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1. Introduction

Today most lattice QCD simulations are performed at unphysical light dynamical quark masses. Chiral perturbation theory (χPT) [1, 2] has proved to be a very important tool for such simulations. By using χPT, one can extrapolate physical quantities to physical light quark masses and get information on low energy constants (LECs) of the chiral theory. Although three-flavor χPT has been successfully used for simulations with 2+1 dynamical quarks, we are still interested in the two-flavor χPT for the following reasons: 1) Usually the simulated light quark masses are much smaller than the simulated strange quark mass. We expect the SU(2) expansion to serve as a better approximation and to converge faster than the SU(3) one. 2) Fits to SU(2) χPT can give us direction information about LECs in the two-flavor theory. 3) By comparing results for SU(2) and SU(3) fits, one can study the systematic errors from truncations of different versions of χPT.

In this work, we study the SU(2) χPT for staggered fermions in the partially-quenched case, and obtain relations between SU(2) and SU(3) LECs by comparing formulae for the pion mass and decay constant from SU(2) and SU(3) χPT. Then, we perform a systematic NNLO SU(2) chiral analysis for recent MILC data in the light pseudoscalar sector. Results for the pion decay constant, SU(2) LECs and chiral condensate in the two-flavor chiral limit are presented.

2. Rooted SU(2) staggered chiral perturbation theory

For lattice simulations based on the staggered fermion formalism, the correct effective theory is rooted staggered χPT (rSXPT) [3, 4, 5, 6, 7], in which taste-violating effects at finite lattice spacings are incorporated systematically. Physical quantities expressed in rSXPT become joint expansions in both $m_q$ and $a^2$, where $a$ is the lattice spacing. The three-flavor rSXPT has been well established [4] and successfully applied in analyzing the lattice data. Here we concentrate on the two-flavor case. Instead of the three-flavor chiral limit $m_u = m_d = m_s = 0$, we perform the expansion around the two-flavor chiral limit $m_u = m_d = 0, m_s = m_s^{phys}$, where $m_s^{phys}$ is the physical strange quark mass.

The SU(2) rSXPT can be constructed by following the same procedure used for SU(3) rSXPT [4]: First, one writes down the Symanzik effective theory (SET) for staggered fermions. Second, one maps the terms in the SET to operators in the chiral Lagrangian by using a spurion analysis. The power counting rule depends on the specific version of staggered fermions being used. For asqtad staggered fermions, we use $a^2 \delta \sim 2Bm \sim p^2$ where $\delta$ is a typical taste-splitting term.

At leading order ($O(a^2, p^2, m_q)$), the chiral Lagrangian for SU(2) SXPT is

$$\mathcal{L}^{(4)} = \frac{f_{(2)}^2}{8} \text{Tr}(D_\mu \Sigma D_\mu \Sigma^\dagger) - \frac{f_{(2)}^2}{8} \text{Tr}(\chi \Sigma^\dagger + \chi \Sigma)$$

$$+ \frac{2\tilde{m}_0^2}{3} (D_{I}^{11} + \ldots + D_{I}^{m_n m_0} + D_{I}^{11} + \ldots + D_{I}^{m_n m_0})^2 + a^2 \mathcal{V'},$$

$$\chi = 2\mu_{(2)} \text{Diag}(m_{I I'}, \ldots, m_{I I'}, m_{I I'}, \ldots, m_{I I'}, m_{I I'}, \ldots, m_{I I'}, m_{I I'}, \ldots, m_{I I'}),$$  \hspace{1cm} (2.1)

where $\Sigma = \exp(r\Phi/f)$ and $\mathcal{V'}$ is the LO taste-violating potential. Their definitions can be found in Ref. [8]. In Eq. (2.1), the replica method is used explicitly: we take $n'_r$ copies of each valence
quark and \( n_r \) copies of each sea quark. At the end of the calculations, we set \( n_r' = 0 \) to account for partial-quenching, and \( n_r = 1/4 \) for taking the fourth-root of the fermion determinants.

At NLO, the SXPT chiral Lagrangian contains two parts: the continuum terms at order \( O(p^4, p^2 m_q, m^2) \) and taste-violating terms at order \( O(p^3 a^2, m_q a, a^4) \). In the partially-quenched case, the NLO continuum SU(2) chiral Lagrangian reads:

\[
\mathcal{L}^{(6)}_{\text{cont}} = -\frac{\rho_0}{4} \left[ \text{Tr}(D_{\mu} \Sigma^\dagger D_{\mu} \Sigma) \right]^2 - \frac{\rho_0}{4} \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \\
+ \rho_0 \left( \text{Tr}(D_{\mu} \Sigma^\dagger D_{\mu} \Sigma D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) - \frac{1}{2} \left[ \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \right]^2 \right) \\
+ \rho_0 \left( \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) + 2 \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \\
- \frac{1}{2} \left[ \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \right]^2 - \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \right) \\
- \frac{\rho_0 + \rho_4}{16} \left[ \text{Tr}(\chi \Sigma^\dagger + \Sigma \chi^\dagger) \right]^2 + \frac{\rho_0}{8} \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \text{Tr}(\chi \Sigma^\dagger + \Sigma \chi^\dagger) \\
+ \frac{\rho_0}{16} \left( \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma (\chi \Sigma^\dagger + \Sigma \chi^\dagger)) - \frac{1}{2} \text{Tr}(D_{\mu} \Sigma^\dagger D_{\nu} \Sigma) \text{Tr}(\chi \Sigma^\dagger + \Sigma \chi^\dagger) \right) \\
+ \frac{\rho_0}{16} \left( 2 \text{Tr}(\Sigma^\dagger \chi \Sigma^\dagger + \Sigma \chi^\dagger ) - \text{Tr}(\chi \Sigma^\dagger + \Sigma \chi^\dagger)^2 - \text{Tr}(\chi \Sigma^\dagger - \Sigma \chi^\dagger)^2 \right) \\
+ \frac{\rho_2}{16} \left[ \text{Tr}(\chi \Sigma^\dagger - \Sigma \chi^\dagger) \right]^2 \\
- \frac{\rho_0}{2} \text{Tr}(\Sigma^\dagger F_{R,\mu \nu} \Sigma F_{L,\mu \nu}) - \frac{i \rho_0}{2} \text{Tr}(F_{L,\mu \nu} D_{\mu} \Sigma^\dagger D_{\nu} \Sigma + F_{R,\mu \nu} D_{\mu} \Sigma D_{\nu} \Sigma^\dagger),
\]

where \( \rho_0 - \rho_3 \) are bare LECs in ordinary SU(2) XPT, and \( \rho_0 - \rho_4 \) are four new (bare) LECs in SU(2) PQXPT. Operators associated with \( \rho_0 \) are unphysical operators, in the sense that physical matrix elements of these operators vanish in the limit where the valence quark masses are set equal to sea quark masses. The specific form of the NLO taste-violating terms are not relevant to this work, so we do not list them here. For more details, please see Ref. [10].

With the LO and NLO SU(2) SXPT Lagrangian, one can calculate the pion mass and pion decay constant in the partially-quenched case. Throughout this work, we always assume that the fourth-root procedure is legitimate [11, 8], and in practice it is done by setting \( n_r = 1/4 \) at the end of the calculations. The results are

\[
\frac{m_{p^+}^2}{(m_\pi + m_\eta)} = \mu_2 \left\{ 1 + \frac{1}{16 \pi^2 f_2^2} \sum_j R_j^{[2,1]} \left( \{ \mathcal{M}_{XY_i}^{[2]} \} \right) l(m_j^2) \\
- 2a^2 \delta_j^{[2]} \sum_j R_j^{[3,1]} \left( \{ \mathcal{M}_{XY_i}^{[3]} \} \right) l(m_j^2) + (V \leftrightarrow A) + a^2 \left( \tilde{L}_2 + \tilde{L}_2' \right) \\
+ \frac{\mu_2}{f_2^2} (4a_2 + p_2 + 4p_2) (m_u + m_d) + \frac{\mu_2}{f_2^2} (-p_1 - 4p_2) (m_\pi + m_\eta) \right\},
\]
Then applying Eq. (2.5) in the NLO formulae of SU(2) staggered ChPT, we get the relations between LO taste-violating parameters and SU(2) LECs by comparing these two sets of formulae. First, by comparing LO meson masses that the expansion has the same pattern as the SU(2) formulae. Furthermore, one can relate SU(3) theory to be generated from the SU(3) theory [1]. This can be seen by expanding the SU(3) staggered ChPT of NLO taste-violating parameters. Definitions for meson masses and residue functions can be found in Ref. [9]. All LECs in Eqs.(2.3) and (2.4) are one-loop renormalized.

In the limit where the light valence quark masses, light sea quark masses and taste-splittings are all small compared to the strange quark mass, i.e., \( m_1, m_2, m_3, m_s \ll m_s \), \( \frac{\Delta a}{\mu_{ms}} \sim \epsilon \ll 1 \), we expect that SU(2) theory to be generated from the SU(3) theory [9]. This can be seen by expanding the corresponding SU(3) formulae [9] for \( m_s^2/(m_s + m_s) \) and \( f_\pi \) in powers of \( \epsilon \). Indeed, one can check that the expansion has the same pattern as the SU(2) formulae. Furthermore, one can relate SU(3) and SU(2) LECs by comparing these two sets of formulae. First, by comparing LO meson masses in various taste channels, we get the relations between LO taste-violating parameters

\[
a^2 \delta^{(2)}_B = a^2 \Delta_B, \quad a^2 \delta'^{(2)} = a^2 \delta'_B, \quad a^2 \delta_A^{(2)} = a^2 \delta_A' .
\]

Then applying Eq. (2.5) in the NLO formulae of \( m_s^2/(m_s + m_s) \) and \( f_\pi \), and comparing coefficients of terms \( m_s, m_s, m_s \) and \( a^2 \) separately, one obtains the following relations [9]:

\[
f(2) = f(1 - \frac{1}{16\pi^2} f(2) \mu_{ms} \log \frac{\mu_{ms}}{\Lambda^2} + \frac{16L_4}{f^2} \mu_{ms}),
\]

\[
\mu(2) = \mu(1 - \frac{1}{48\pi^2} f(2) \frac{4\mu_{ms}}{3} \log \frac{\mu_{ms}}{\Lambda^2} + \frac{32(2L_6 - L_4)}{f^2} \mu_{ms}),
\]

\[
p_1 = 16L_5 - \frac{1}{16\pi^2} (1 + \log \frac{\mu_{ms}}{\Lambda^2}),
\]

\[
p_2 = -8L_8 + \frac{1}{16\pi^2} \frac{1}{6} (\log \frac{4\mu_{ms}}{\Lambda^2}) + \frac{1}{16\pi^2} \frac{1}{4} (1 + \log \frac{\mu_{ms}}{\Lambda^2}),
\]

\[
l_3 = 8(2L_6 - L_4) + 4(2L_6 - L_5) - \frac{1}{16\pi^2} \frac{1}{36} (1 + \log \frac{4\mu_{ms}}{\Lambda^2}),
\]

\[
l_4 = 8L_4 + 4L_5 - \frac{1}{16\pi^2} \frac{1}{4} (1 + \log \frac{\mu_{ms}}{\Lambda^2}),
\]

\[
\tilde{L}_2 = \tilde{L} - \frac{1}{6} \tilde{D} (1 + \log \frac{4\mu_{ms}}{\Lambda^2}) - \frac{1}{2} \tilde{D} (1 + \log \frac{\mu_{ms}}{\Lambda^2}),
\]

\[
\tilde{L}_2 = \tilde{L} - \frac{1}{6} \tilde{D} (1 + \log \frac{4\mu_{ms}}{\Lambda^2}) + \frac{1}{2} \tilde{D} (1 + \log \frac{\mu_{ms}}{\Lambda^2}),
\]

Here, \( \delta_B^{(2)} \) and \( \delta'_B^{(2)} \) are LO taste-violating parameters, and \( L_2'' \) and \( \tilde{L}_2 \) are linear combinations of NLO taste-violating parameters. Definitions for meson masses and residue functions \( R \) and \( D \) can be found in Ref. [9]. All LECs in Eqs.(2.3) and (2.4) are one-loop renormalized.
where \( L_4, L_5, L_6 \) and \( L_8 \) are renormalized SU(3) LECs, and \( \tilde{L}' \) and \( \tilde{L}'' \) are the NLO taste-violating parameters in SU(3) rSZPT. Equations (2.10) and (2.11) are the same as the equations in the full QCD continuum case [1]. Equations (2.8) and (2.9) relate the unphysical LECs in the partially-quenched two-flavor theory to the physical LECs in the three-flavor theory. Equations (2.12) and (2.13) give us relations between taste-violating parameters in the two-flavor and three-flavor theories.

3. SU(2) chiral analysis of the MILC data

Currently, we have gauge ensembles generated from 2+1 dynamical simulations using asqtad staggered fermions. Lattice spacings range from 0.15 fm to 0.045 fm. The light pseudoscalar mass and decay constant are measured with different combinations of valence and sea quark masses. With these data, we perform a systematic NNLO SU(2) chiral analysis by using the NNLO formulae for \( m_\pi^2 \) and \( f_\pi \). Results of physical quantities are updated from the previous analysis in Ref. [12].

The NNLO formulae for \( m_\pi^2/(m_x + m_y) \) and \( f_\pi \) are obtained by combining the NLO formulae Eqs. (2.3) and (2.4), possible analytic NNLO terms and the continuum NNLO chiral logarithms provided by Bijnens and Lähde [13]. The root mean square (RMS) average pion mass is used in NNLO chiral logarithms. In order for the SU(2) formulae to apply, we require both the valence and sea light quark masses to be significantly smaller than the strange quark mass. In practice, we used the following cutoff on our data sets: \( m_t \leq 0.2m_s, m_x + m_y \leq 0.5m_s, \text{max}(m_x, m_y) < 0.3m_s \). Furthermore, in order for the continuum NNLO chiral logarithms to be applicable, we also require the taste-splittings between different pion states to be significantly smaller than the kaon and pion masses. The lattices that are at least close to satisfying these conditions are fine (\( a \approx 0.09 \) fm), superfine (\( a \approx 0.06 \) fm) and ultrafine (\( a \approx 0.045 \) fm) lattices. In practice, we used superfine and ultrafine lattices for our central value fit, and we included fits to all three kinds of lattices to estimate systematic errors. One difference from the previous fit is that this time we used modified quark masses \( m \rightarrow \tilde{m} = m + a^2/(2\mu) \) in NNLO analytic terms to make the NNLO LECs scale invariant on the lattice, not just in the continuum.

4. Results

For the central fit, we used three superfine ensembles \((am_l,am_s)\) = \{\(0.0018,0.018\), \(0.0025,0.018\), \(0.0036,0.018\)\} and one ultrafine ensemble \((am_l,am_s)\) = \(0.0028,0.014\). There are a total of 50 data points and 30 parameters with appropriate constraints. This fit has a \( \chi^2 \) of 18 with 20 degrees of freedom, giving a confidence level CL \( \approx 0.6 \). The volume dependence at NLO has been included in the fit formulae, and a small (\( \leq 0.3\% \)) residual finite volume correction [14, 8] is applied at the end of the calculations.

In Fig. 1 we show the fit results for the light pseudoscalar mass and decay constant as functions of the sum of the quark masses \( m_x + m_y \). The red solid curve represents the full NNLO results for full QCD in the continuum case, where we have set the taste-splittings and taste-violating parameters to zero, extrapolated to \( a = 0 \) linearly in \( \alpha_s a^2 \), and set valence and sea quark masses equal. The continuum results through NLO and LO are shown in blue and magenta curves respectively.

Finally, we find the physical values of the average up and down quark mass \( \bar{m} \) by requiring that \( \pi \) has its physical mass, and then find the decay constant corresponding to this point.
SU(2) staggered ChPT

Figure 1: SU(2) chiral fits to $f_\pi$ (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.

In Fig. [a], with the scale $r_1 = 0.3133(23)$ fm determined by HPQCD [15], we obtain $f_\pi = 130.2 \pm 1.4 \left( ^{+2.0}_{-1.6} \right)$ MeV, where the first error is statistical and the second error is systematic. This agrees with the PDG 2010 value $f_\pi = 130.4 \pm 0.2$ MeV [16]. Alternatively, one can fix the scale by using the SU(3) NNLO result of $f_\pi$ [17]. We then obtain

$$f_2 = 123.8 \pm 1.4 \left( ^{+1.0}_{-1.7} \right) \text{ MeV}$$
$$I_3 = 2.85 \pm 0.81 \left( ^{+0.37}_{-0.92} \right)$$
$$I_4 = 3.98 \pm 0.32 \left( ^{+0.51}_{-0.28} \right)$$
$$\hat{m} = 3.19(4)(5)(16) \text{ MeV}$$
$$\langle \bar{u}u \rangle_2 = -[281.5(3.4) \left( ^{+2.0}_{-2.9} \right) (4.0) \text{ MeV}]^3 \quad (4.1)$$

The quark masses and chiral condensate are evaluated in the $\overline{MS}$ scheme at 2 GeV. We used the two-loop perturbative renormalization factor [18] to do the conversion. Errors from perturbative calculations are listed as the third errors in these quantities. All the quantities agree with SU(3) results [17] within errors.

5. Discussion and outlook

In this work, we studied SU(2) rSXPT in the partially-quenched case, and we performed a systematic SU(2) chiral analysis for recent asqtad data in the light pseudoscalar sector. Results for SU(2) LECs, decay constant and chiral condensate in the chiral limit are in good agreement with results from an SU(3) analysis [17]. It can be seen that the SU(2) theory within its applicable region converges much faster than the SU(3) one. For the point $x = 0.05$ on the x-axis in Fig. [a], the ratio of the NNLO correction to the result through NLO is 1% both for $f_\pi$ and $m_\pi^2/(m_x + m_y)$. In contrast, the same ratio in SU(3) analysis is 3% for $f_\pi$ and 15% for $m_\pi^2/(m_x + m_y)$, respectively, although the large correction in the mass case is partly the result of an anomalously small NLO term.
Since the simulated strange quark masses vary slightly between different ensembles, parameters in SU(2) \(\chi PT\) should also change with ensembles. In this work, we also tried to include this effect by using the adjustment formulae in Ref. [9]. It turns out that the fits are improved, but not significantly. This part may still need further investigation, hence we do not include these results in this work.

In the future, a next step is to include the kaon as a heavy particle in SU(2) \(\chi PT\) in order to study physics involving the strange quark, e.g., the kaon mass and decay constant. This method has been used in Ref. [19]. Another step is to extend the analysis to data obtained from simulations with HISQ fermions, where taste-violating effects are further reduced. This can be done using the same approach as soon as the data are available.

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