NLO and NNLO chiral fits for 2+1 flavor DWF ensembles

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We study the use of NLO and NNLO formulae from SU(2) chiral perturbation theory to fit results from the 2+1 flavor DWF QCD ensembles that have been generated by the RBC and UKQCD collaborations. These ensembles are at two different lattice spacings, contain multiple dynamical light quark masses, and include a variety of partially quenched valence quark masses. Both NLO and complete NNLO fits well represent our data, which has m_π in the range 220 to 420 MeV. With our data, the NNLO fits have NLO and NNLO contributions of similar size, making the series not convergent and the extrapolation to physical light quark masses imprecise. Thus, we use NLO fit results for our predictions of f_π, f_K and the light quark masses.

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1. Introduction

The RBC and UKQCD Collaborations have been generating 2+1 flavor domain wall fermion (DWF) QCD ensembles over the last few years. Extensive results have been published from the first ensemble, which had two dynamical quark masses, a variety of valence quark masses, $1/a = 1.72(2)$ GeV and a spatial volume of $(2.75 \text{ fm})^3$ [1, 2, 3]. The largest sources of systematic errors in these results are the $O(a^2)$ errors and errors from extrapolating from our simulation light quark masses to the physical light quark masses. We estimated both of these to be about 4% for f_π, for example. We now have a second ensemble at a smaller lattice spacing, which allows us to extrapolate to $a = 0$, assuming that our data is in the region where the errors are of $O(a^2)$. The second ensemble also has lighter dynamical quarks and allows us to probe the reliability of the chiral extrapolation for our data. This report details our analysis of the combined data from both ensembles, including chiral and continuum extrapolations.

The details of our ensembles are given in Table 1. For the results from our $1/a = 1.72$ GeV ensembles given in [1], measurements were made on ensembles of length 3600 MD time units (after thermalization). We have generated more lattices, so that for the $1/a = 1.72$ GeV ensemble with light quark mass $m_l = 0.005$, our results come from 8080 MD time units and for the heavier light quark mass, $m_l = 0.01$, 7180 time units. This more than doubles the measurements from our earlier work. For the $1/a = 2.32$ GeV ensemble, we have 6100 MD time units, after thermalization, for $m_l = 0.004$, 6220 for $m_l = 0.006$, and 5020 for $m_l = 0.008$.

The analysis we present here uses our measurements of light-light pseudoscalar masses (pions), strange-light pseudoscalar masses (kaons) and the mass of the Ω baryon, m_Ω to set the lattice scale and determine the physical light and strange quark masses (we assume $m_u = m_d$ throughout). As inputs, we take the known values for m_π, m_K and m_Ω. We have also measured the light-light and light-strange pseudoscalar decay constants, and predictions for these are an output of our analysis and a check on our systematic errors. A major focus of our analysis is how well full NLO and NNLO chiral perturbation theory formulae fit our data and whether the apparent convergence of the series and estimates of the size of neglected terms are consistent with general theoretical estimates and known values for f_π and f_K.

2. Observables, reweighting and global fits

For light-light and heavy-light pseudoscalars, we use Coulomb gauge fixed wall source propagators. We fit the propagators starting at 10 lattice spacings from the wall source and find no dependence on this choice of fit range. The plateaus are very long for these states - we fit over 44 lattice spacings for both ensembles. Coulomb gauge fixed box sources are used for the Ω, with a box size of 16^3 for the $1/a = 1.72$ GeV ensemble and 20^3 for the 2.32 GeV ensemble. These sources also give very good signals, and we fit over a range of 7 lattice spacings. We find statistical errors on the pseudoscalar masses and decay constants in the range of 0.2-0.5%, and errors on m_Ω of 0.2-0.7%.

With these measurements, we then fit our data to SU(2) chiral perturbation theory (ChPT) formulae. With SU(2), we do not assume that m_s (or alternatively m_K) is small. We do need

Ensemble	$(m_l^{\text{lat}}, \widetilde{m}_l)$	m_π (MeV)	$(m_{\text{val}}^{\text{lat}}, \widetilde{m}_{\text{val}})$	m_π^{val} (MeV)
$1/a = 1.72(2)$ GeV			(0.001, 11.2 MeV)	239
$24^3 \times 64 \times 16$			(0.005, 22.0 MeV)	328
$(2.75 \text{ fm})^3$			(0.010, 35.5 MeV)	417
$m_h^{\text{lat}} = 0.04$	(0.005, 22.5 MeV)	328	(0.020, 62.5 MeV)	
$\widetilde{m}_h = 116.5$ MeV	(0.01, 35.5 MeV)	417	(0.030, 89.5 MeV)	
$m_{\text{res}}^{\text{lat}} = 0.00315$			(0.040, 116.5 MeV)	
$m_{\text{res}} = 8.5$ MeV				
$1/a = 2.32(3)$ GeV			(0.002, 9.83 MeV)	226
$32^3 \times 64 \times 16$			(0.004, 17.2 MeV)	295
$(2.72 \text{ fm})^3$	(0.004, 17.2 MeV)	295	(0.006, 24.6 MeV)	350
$m_h^{\text{lat}} = 0.03$	(0.006, 24.6 MeV)	350	(0.008, 32.0 MeV)	397
$\widetilde{m}_h = 113.1$ MeV	(0.008, 32.0 MeV)	397	(0.025, 94.7 MeV)	
$m_{\text{res}}^{\text{lat}} = 0.000664$			(0.030, 113.1 MeV)	
$m_{\text{res}} = 2.45$ MeV				

Table 1: Run parameters for the simulations presented here. Quark and pion masses are given in MeV. Quark masses are reported in $\overline{\text{MS}}(2 \text{ GeV})$, which uses the lattice spacings we determine from our analysis and a separate NPR measurement of the quark mass renormalization factors. The notation is as in [1] – in particular, quark masses with a tilde are total quark masses.

$m_l \ll m_s$. For the light-strange sector, we use SU(2) for kaons, as we did in [1]. In our SU(2) fits, we include $O(a^2)$ corrections to leading order LEC's, and neglect any a^2 dependence for NLO, or higher, LEC's. The residual mass effects of DWF are taken into account by including the contribution of m_{res} in the total quark mass.

Of course, there are many ways to write down SU(2) ChPT formula at NLO, since any rearrangement of the series that only changes it at NNLO is equally valid. Since we have no *a priori* reason to know which particular ordering is the most convergent for a particular quantity, and it may seem unlikely that any one reordering will be optimal for all quantities, we use the series as an expansion in f, the chiral limit value for the pion decay constant. The pseudoscalar masses that enter at NLO and higher are just $m^2 = 2Bm_q$, the leading order expressions. This view of the series also readily extends to the full, continuum NNLO forms, as given in [4].

Since the total lattice quark mass enters into the ChPT expressions and we are working at two different lattice spacings, we need a renormalization factor to relate bare quarks at one lattice spacing to the other. We have gotten this ratio three different ways: 1) from NPR calculations at the two different lattice spacings, 2) from matching the two lattice spacings at unphysical quark masses [6] and 3) from a global fit where the ratio is a free parameter and it is fit for in an overall χ^2 minimization step. All three methods agree within their errors.

A last issue in our global fits is the difference between the dynamical heavy quark mass in the simulations, m_h, and the physical strange quark mass, m_s. When the simulations are run, the value of m_h to use is not known. Only after a complete analysis of the data does one gain knowledge about the correct value of m_h. In SU(2) ChPT, unlike SU(3), all LEC's are implicit functions of m_h and cannot be extrapolated to the physical value. (For valence heavy quark mass dependence,

it is easy to interpolate between the values for a hadron mass that are measured with different valence quark masses to a self-consistently determined strange quark mass.) By reweighting our observables from the simulated m_h to the desired m_s, we can remove any systematic error from the (generally mild) dependence on m_h.

The left graph in Figure 1 shows the unitary values for f_π as a function of the reweighted dynamical heavy quark mass for three of our ensembles. The right graph shows the ratio of the reweighted value of f_π to the unreweighted value for the $1/a = 2.32$ GeV, 0.004/0.03 ensemble. Four stochastic estimators per mass step were used here and studying the reweighting dependence versus the number of stochastic hits indicates that four are sufficient. We see a clear signal for a small dependence on the strange quark mass. More details of this procedure are also given in [7].

Three different global fits, using the above procedure have been performed by members of our collaboration and the agreement for physical quantities is very good. Two types of fits use results from matching the lattices at unphysical quark masses to constrain the ratio of quark renormalization factors and/or lattice spacings. A third fit self-consistently fits the data, determining the ratio of lattice spacings, quark mass renormalizations and LECs that give the best χ^2. We do uncorrelated fits to our data, since we find our covariance matrices are very singular, due to the data being strongly correlated. As shown in [8] in such a case an uncorrelated fit gives the correct answer, but the quoted χ^2 is not a reliable goodness-of-fit indicator.
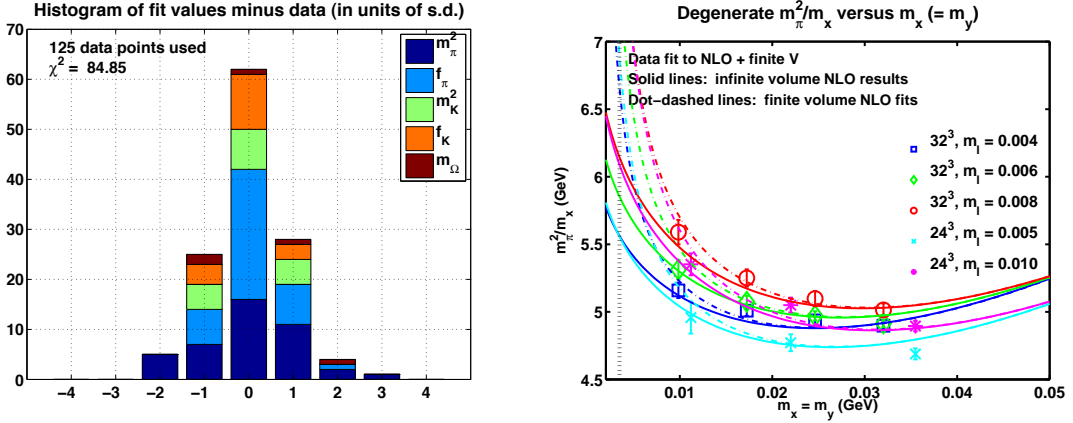
The left graph of Figure 2 shows a histogram of the uncorrelated χ^2 for our fits, which involve 125 data points and about 20 parameters, depending on precisely which fit was done. All of our partially quenched data for light-light and heavy-light pseudoscalars and the Ω are fit simultaneously, under an outer jackknife loop, which produces the errors. The fit is to NLO order in ChPT, including finite volume effects. The physical values for m_π, m_K and m_Ω are used to determine the lattice scale and quark masses. From NPR [5], we use a value of $Z_m = 1.590$ for the $1/a = 2.32$ GeV ensemble to convert lattice quark masses into continuum masses renormalized in $\overline{\text{MS}}(2\,\text{GeV})$. The histogram shows that the fits are in good agreement with the error bars on each data point. The right graph of Figure 2 shows the comparison between the NLO ChPT fit results and the data for pions made of degenerate quarks. Curvature consistent with the expected chiral logarithms is seen.

Figure 3 shows our results for the unitary light-light pseudoscalar decay constant and our fits. We find $f_\pi = 122.2 \pm 3.4_{\text{stat}}$ MeV. The right graph shows the LO and NLO contribution to the fit and one sees that in the region where we have data, the NLO contribution is a 20-30% correction to the LO result. From this one would expect an NNLO error of order 0.2^2 to 0.3^2 or $O(4-9\%)$. One sees that our prediction for f_π is low by roughly this amount. We also estimate a similar ChPT systematic effect by looking at simple, analytic fits to our data [6]. We quote a preliminary ChPT systematic error given by the square of the ratio of NLO to LO in the lightest quark mass region where we have data.

A priori, one has little information about the size of NNLO ChPT contributions. If the series is reasonably convergent when the next order is added, the NNLO terms should be roughly the square of the NLO contributions. Of course ChPT differs from a renormalizable field theory in that many new LEC's enter at the next order, as well as contributions from LEC's at the current order times logarithms. For DWF, where we have continuum chiral symmetries at finite lattice spacing, we can fit our data to the continuum NNLO SU(2) formulae, to help address these questions.
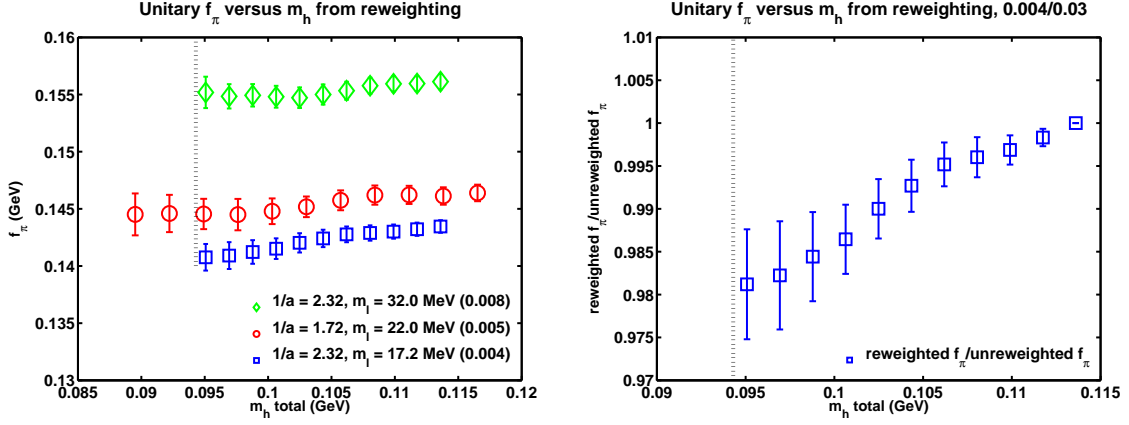
Figure 1: The left graph shows the reweighted value for f_π for some of our ensembles. The right graph is the ratio of f_π, reweighted to the quark mass given on the horizontal axis, to the unreweighted f_π.


Figure 2: The left graph is a histogram of the deviations of fit values from measured values, in units of the σ for the data points. The right graph shows results from the partially quenched, NLO ChPT fits for m_π^2.
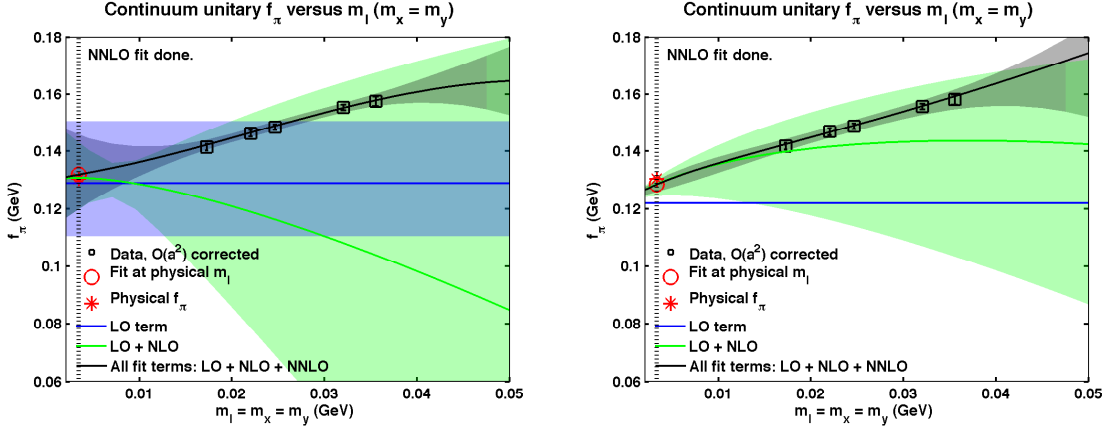
3. Full NNLO fit

We have also fit our data to the full, continuum NNLO ChPT results for SU(2) given by Bijnens and Lahde [4]. This adds 13 new parameters to our fits, five L_i and eight, linearly-independent combinations of the K_i. For now, we have done NNLO fits keeping the lattice spacing and ratio of quark mass renormalization factors fixed to the values returned from NLO fits.

The left graph in Figure 4 shows the results for f_π from a full NNLO fit to all of our partially quenched, light-light masses and decay constants. Both lattice spacings are fit simultaneously using a standard, least-squares approach and the uncorrelated $\chi^2 = 21.8$ with 125 data points and 33 parameters. Statistical errors come from a jackknife analysis. The NNLO fit predicts $f_\pi = 133 \pm 13_{\text{stat}}$ MeV, $f = 130.4 \pm 20.0_{\text{stat}}$ and gives values for m_{ud} and m_s the same, within statistical errors, as the NLO fits. The blue band in the figure gives the one σ error for the LO contribution, the green shows the error for the LO + NLO contribution and the black the error for the LO + NLO + NNLO contribution. The large size of the green error band means that, for the majority of our
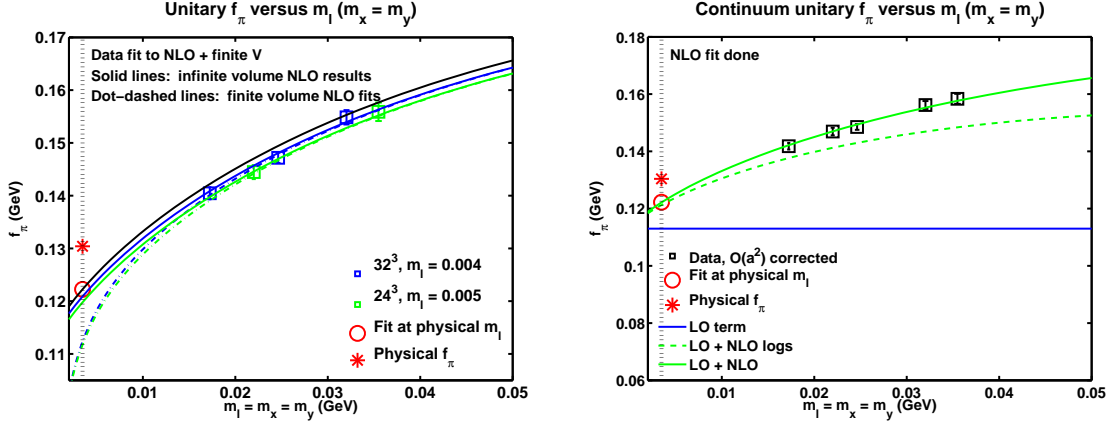
Figure 3: The left graph shows the unitary, light-light pseudoscalar decay constant versus quark mass, from our NLO fit. The right graph shows the contribution of various terms to the fit.

Figure 4: The left graph is f_π from a full NNLO fit to our data. The right graph is also for a full NNLO fit, but with the constraint that the SU(2) chiral limit decay constant, $f = 122.0$ MeV.

fits under the jackknife loop, the size of the NNLO contributions is very large and the series is not convergent. This observation, along with the increase in the statistical error for f_π from the extra degrees of freedom in the fit, means that we cannot get an accurate extrapolation to physical light quark masses by fitting our data, which has $m_\pi = 220$ to 420 MeV, to NNLO order in ChPT.

The right graph in Figure 4 shows the results for f_π from a full NNLO fit, with the constraint that the SU(2) chiral limit decay constant, $f = 122$ MeV. (This value of f comes from the phenomenological value for $\bar{l}_4$ and has an uncertainty of about 1 MeV.) The total, uncorrelated χ^2 for these fits is about 25 and gives $f_\pi = 127.9 \pm 1.8_{\text{stat}}$ MeV. (The smaller statistical error for this fit comes from the strong constraint in the chiral limit.) However, the large error on the LO + NLO contribution, means that, in a $\sim 25\%$ of our fits, we have very large NNLO contributions. Thus we cannot demonstrate a reasonably convergent series at this point, even with a constraint.

4. Summary and Conclusions

We have found that our 2+1 flavor DWF QCD data from two lattice spacings, with partially quenched m_π from 220 to 420 MeV, can be fit with either NLO or full NNLO ChPT formulae. Standard, least-squares fits yield small, uncorrelated values for χ^2, so the fit formulae well represent our data. For unconstrained NNLO fits, we find $f_\pi = 133 \pm 13_{\text{stat}}$ MeV and the series is not convergent. Constraining the chiral limit value for f to be 122.0 MeV gives $f_\pi = 127.9 \pm 1.8_{\text{stat}}$ and the series appears less poorly convergent. With the current data set, NNLO fits do not provide a reliable extrapolation to physical light quark masses.

Turning to NLO fits, we find the NLO terms for f_π are 20-30% the size of the LO term, at quark masses where we have data. From this, we estimate a 4-9% correction due to NNLO terms and our value for f_π deviates from the physical value by about this much. We take the square of the fractional size of the NLO correction as an estimate of our systematic ChPT error. We also have used NPR to determine the quark mass renormalization, allowing us to determine values for m_{ud} and m_s. Our preliminary results are:

$$m_{ud}^{\overline{\text{MS}}}(2\,\text{GeV}) = 3.47 \pm 0.10_{\text{stat}} \pm 0.17_{\text{NPR}}\ \text{MeV}$$
$$m_s^{\overline{\text{MS}}}(2\,\text{GeV}) = 94.3 \pm 3.4_{\text{stat}} \pm 4.5_{\text{NPR}}\ \text{MeV} \qquad m_s/m_{ud} = 27.19 \pm 0.35_{\text{stat}}$$
$$f_\pi = 122.2 \pm 3.4_{\text{stat}} \pm 7.3_{\text{ChPT}}\ \text{MeV}$$
$$f_K = 149.7 \pm 3.8_{\text{stat}} \pm 2.0_{\text{ChPT}}\ \text{MeV} \qquad f_K/f_\pi = 1.225 \pm 0.012_{\text{stat}} \pm 0.014_{\text{ChPT}}$$
$$f = 113.0 \pm 3.8_{\text{stat}} \pm 6.8_{\text{ChPT}}\ \text{MeV}$$
$$f_K^{(0)} = 144.8 \pm 4.2_{\text{stat}} \pm 2.0_{\text{ChPT}}\ \text{MeV} \qquad f_K^{(0)}/f = 1.282 \pm 0.015_{\text{stat}} \pm 0.017_{\text{ChPT}}$$

References

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