

Lattice study of the chiral properties of large- N_c QCD

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We present a lattice calculation of the low energy constants of QCD with $N_c = 3, 4$ and 5 colors and $N_f = 2$ flavors of degenerate mass fermions. We fit data for the pseudoscalar meson mass, the pseudoscalar decay constant, and the axial Ward identity fermion mass to formulas from next-to-next-to leading order chiral perturbation theory. We extract the next to leading order low energy constants and study their behavior as a function of N_c . Preexisting analyses of $N_c = 3$ inform our fitting strategies.

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I. INTRODUCTION AND MOTIVATION

The most studied deformation of real-world three-color ($N_c = 3$) QCD is its extension to a large number of colors. In the limit that N_c is taken to infinity, it is believed that mesons are narrow quark antiquark bound states, baryon masses scale as N_c , and N_c counting rules set the overall scale for hadronic matrix elements [1–3].

There is a small lattice literature related to the large N_c limit of QCD. Simulations involve the pure gauge theory and fermions included in quenched approximation (mostly at single-digit values of N_c), quenched simulations at very large N_c and small volume, and simulations in large volume with a small number of dynamical fermion flavors (so far, $N_f = 2$ and 4). References [4–6] are a selection of reviews of the various approaches. The goal of these simulations is to confront predictions of large N_c QCD, which are typically (semi) analytic, with nonperturbative lattice-based results.

The qualitative situation with regard to such comparisons is as follows: Choose to fix the lattice spacing in a simulation using some observable taken from a correlation function dominated by gluonic degrees of freedom. Such observables include the string tension, the Sommer parameter [7], or the flow [8,9] parameter t_0 . Perform lattice simulations while tuning the bare parameters (the most sensitive one is the gauge coupling g^2) so that the lattice spacing is the same for all values of N_c . One will discover that the bare 't Hooft couplings $\lambda = g^2 N_c$ are roughly matched across N_c . Alternatively, performing simulations across N_c at the same value of λ , one will discover that the

lattice spacing had been approximately matched. Once that is done one will see that the masses of flavor nonsinglet mesons, and their dependence on the fermion mass, will be approximately equal across N_c . Simple matrix elements (decay constants, the kaon $B-$ parameter) will scale with N_c as predicted from the color weight of amplitudes. All of these statements are modified by small corrections, which can be arguably interpreted as $1/N_c$ effects.

We are not aware of any large volume simulations which attempt to take a continuum limit; most of them involve simulations across N_c at a single matched value lattice spacing. It seemed to us that it might be possible to extend one of these studies to do that. We make a first attempt to measure at chiral parameters of $SU(N_c)$ gauge theory with $N_f = 2$ flavors of degenerate fermions, in the continuum and large N_c limits. Specifically, we studied $N_c = 3, 4$ and 5. We wanted to address the following set of questions:

- (1) How do the low energy constants of the chiral effective theory scale with N_c ?
- (2) What is their $N_c \rightarrow \infty$ limit? How do our results compare to those from other approaches (quenched simulations, simulations in small volume)?
- (3) As N_c rises, the low energy effective theory is expected to change from the conventional $SU(N_f)_L \times SU(N_f)_R \rightarrow SU(N_f)_{L+R}$ pattern of symmetry breaking to one where the flavor singlet meson becomes light [10–15]. At what value of N_c does this “ $U(N_f)$ ” expansion begin to reproduce the data?

There is already an extensive literature about the low energy constants of $N_c = 3, N_f = 2$ QCD, summarized in the Flavor Lattice Averaging Group’s 2019 summary, Ref. [16]. Typical analyses in their summary have much better quality than what we present here; we cannot add much to this already-closed subject. We instead use the results of these pre-existing $N_c = 3, N_f = 2$ studies to inform our analysis, and to calibrate the accuracy we claim for $N_c > 3$.

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We should say at the start that while we have made a first attempt to extract continuum to the low energy constants of $N_c > 3$ QCD, we do not regard our results as definitive. The main issues are three: two typical of early QCD studies of any observable, with too large a lattice spacing and too large fermion masses for comfortable extrapolations, the third is that we do not feel that we have enough values of N_c . But the outline of the solution is there: once again, $N_c = 3$ is not that different from infinite N_c .

Our calculation was strongly influenced by two previous ones. The first is a 2013 computation of the low energy parameters of $N_f = 2$ QCD ($N_c = 3$) in the continuum limit, by the Budapest-Marseille-Wuppertal collaboration [17]. Their study has larger volumes, smaller lattice spacings, and smaller fermion masses than our exploratory project. We adapted much of their analysis methodology. The other project was a calculation of the low energy parameters of $N_f = 4$ systems by P. Hernández, C. Pena and F. Romero-López [18]. This was done at a single lattice spacing, matched across N_c . They studied $N_c = 3, 4, 5$, and 6. The addition of $N_c = 6$ allowed for more controlled extrapolation to infinite N_c than we could do. This is because large N_c predictions typically involve a power series in N_c :

$$\langle O(N_c) \rangle = c_0 + \frac{c_1}{N_c} + \frac{c_2}{N_c^2} + \dots \quad (1)$$

and it is useful to have more than $j + 1$ values of N_c to fit data to such predictions at j th order.

Most discussions of the literature of large N_c QCD (such as the one we just gave) make the point that comparisons across N_c reveal only small differences. But to lattice practitioners QCD's at different N_c 's are different. Some of these differences are unfavorable. For example, the up-front cost of a simulation at some N_c scales roughly like N_c^2 (when matrix times vector multiplication dominates, a situation encountered in inverting the Dirac operator) or N_c^3 (for matrix multiplication of gauge links). The simulation autocorrelation time as measured by the topological susceptibility grows with N_c , in both quenched simulations and ones with dynamical fermions.

However, differences across N_c can be favorable for larger N_c . That is the case in this project, where we had much greater difficulty generating useful $N_c = 3$ datasets than we did with $N_c = 4$ or 5. This is due to the scaling of the pseudoscalar decay constant F with N_c : $F \propto \sqrt{N_c}$. This is helpful in two (related) ways. First, the expansion parameter of chiral perturbation theory is (speaking loosely) the ratio of the squared pseudoscalar mass to F^2 , $x = m_{\text{PS}}^2 / (8\pi^2 F^2)$. Simulations which make comparisons at identical x across N_c involve ever larger values of m_{PS}^2 and become easier to perform as N_c grows. Second, finite volume corrections in a box of size L are proportional to $\Delta(m_{\text{PS}}, L) / F^2$ where $\Delta(m_{\text{PS}}, L)$ is the propagator of a

pseudoscalar “to an image point,” which appears along with the “tadpole” or “snail” graph in finite volume. The $1/F^2 \propto 1/N_c$ prefactor means that as N_c grows there are smaller finite volume corrections at identical pion masses. As a consequence, at bigger N_c one can simulate at smaller volume without encountering volume artifacts.

The outline of the paper is as follows: Sec. II sets the conventions we follow for the low energy chiral effective theory, to which we compare our data. Sections III and IV describe the various parts of the lattice simulation, first the collection of data and its conversion to the dimensionless quantities which are what we fit, and then a discussion of issues involved in the fits themselves. Results of fits which extract the low energy constants of the chiral effective Lagrangian are presented in Sec. V. Some conclusions are found in Sec. VI.

II. THEORETICAL BACKGROUND AND CONVENTIONS FOR CHIRAL OBSERVABLES

The goal of this project is to compare the relationship between quantities relevant to the low energy properties of $SU(N_c)$ gauge theory with two flavors of degenerate mass fundamental representation fermions, across N_c and in the continuum limit. We focus on the fermion mass, the (squared) pseudoscalar mass and pseudoscalar decay constant as measured in simulations. We label these quantities as m_q , m_{PS}^2 , and f_{PS} . The comparisons are done in the context of the parameters of a low energy effective chiral Lagrangian. There are two choices for an effective theory, which differ in the number of light degrees of freedom they represent.

The effective field theory for $N_c = 3$ QCD is based on the spontaneous breaking of chiral symmetry $SU(N_f)_L \times SU(N_f)_R \rightarrow SU(N_f)_{L+R}$ (plus its explicit breaking by quark masses). Its small expansion parameter is

$$O(\delta) \sim O(p^2) \sim O(M^2) \sim O(m_q) \quad (2)$$

where M^2 is the squared mass of the fields in the Lagrangian (taken to be massless Goldstone bosons in the $m_q \rightarrow 0$ limit). We will refer to this effective theory as “ $SU(N_f)$ effective theory.” (Of course, for us, $N_f = 2$.)

Only flavor nonsinglet mesons appear in the Lagrangian of $SU(2)$ effective theory. In particular, the flavor singlet meson, the eta-prime (in $N_f = 3$ language) gets a large mass from the anomaly and does not appear in the low energy theory of the $N_c = 3$ world.

However, the situation at large N_c is different. The size of anomaly term falls with N_c and the squared eta prime mass decreases as $1/N_c$, so at some point the eta prime must be included in the low energy effective theory. The resulting theory is called $U(N_f)$ [here $U(2)$] effective theory and has a slightly different chiral expansion.

Which chiral expansion scheme works better for any particular value of N_c is an open question, which we hope to explore.

We begin by discussing $SU(2)$ chiral perturbation theory. We follow the usual convention for lattice simulations and define the pseudoscalar decay constant f_{PS} in terms of the matrix element

$$\langle 0 | \bar{u} \gamma_0 \gamma_5 d | \pi \rangle = m_{\text{PS}} f_{\text{PS}}. \quad (3)$$

This leads to the identification $f_\pi \sim 132$ MeV in QCD. Note that the continuum chiral PT literature uses a “93 MeV” definition: the extra $\sqrt{2}$ is an isospin raising factor. See Ref. [19] for a compilation of conventions for this quantity.

There are two commonly used expansion schemes for $SU(N_f)$ chiral perturbation theory. The two leading order constants are B and F . We will mostly use the “ x -expansion” which is given in terms of m_q via the quantity

$$x = \frac{M^2}{8\pi^2 F^2}, \quad (4)$$

where $M^2 = 2Bm_q = 2\Sigma m_q/F^2$ and Σ is the fermion condensate. Note that x is $O(\delta)$ according to Eq. (2). In next to leading order (NLO), Bijens and Lu [20] define (converting F conventions)

$$\bar{A}(M^2) = \frac{M^2}{8\pi^2} \log \frac{\mu^2}{M^2} \quad (5)$$

and the formulas to be addressed are

$$\begin{aligned} m_{\text{PS}}^2 &= 2Bm_q \left[1 + \frac{a_M}{F^2} \bar{A}(M^2) + \frac{M^2}{F^2} b_M + \dots \right] \\ f_{\text{PS}} &= F \left[1 + \frac{a_F}{F^2} \bar{A}(M^2) + \frac{M^2}{F^2} b_F + \dots \right]. \end{aligned} \quad (6)$$

Here

$$\begin{aligned} a_M &= -\frac{1}{N_f} \\ b_M &= 8N_f(2L_6 - L_4) + 8(2L_8 - L_5) \\ a_F &= \frac{1}{2}N_f \\ b_F &= 4(N_f L_4 + L_5). \end{aligned} \quad (7)$$

The L_i 's are the low energy constants (LEC's) of the NLO chiral expansion. The b_j 's depend on the choice of scale in the logarithm of $\bar{A}(M^2)$.

The FLAG review [16] and Ref. [17] make a slightly different definition, which we will employ:

$$\frac{a_j}{F^2} \bar{A}(M^2) + \frac{M^2}{F^2} b_j \equiv a_j \frac{M^2}{8\pi^2 F^2} \left[\log \frac{\mu^2}{M^2} + l_j \right]. \quad (8)$$

The l_i 's are scheme (μ^2) dependent, while B and F are not. Note that

$$l_i(\mu_2) = l_i(\mu_1) + \log \frac{\mu_1^2}{\mu_2^2}. \quad (9)$$

The convention is that b_M is replaced by l_3 and b_F is replaced by l_4 .

We will actually need the next-to next-to leading order (NNLO) expression:

$$\begin{aligned} m_{\text{PS}}^2 &= 2Bm \left[1 - \frac{1}{2}x \left(\ln \frac{\mu^2}{M^2} + l_3 \right) + x^2 \left(\frac{17}{8}T_M^2 + k_M \right) \right] \\ f_{\text{PS}} &= F \left[1 + x \left(\ln \frac{\mu^2}{M^2} + l_4 \right) + x^2 \left(-\frac{5}{4}T_F^2 + k_F \right) \right], \end{aligned} \quad (10)$$

where

$$\begin{aligned} T_M &= \ln \frac{\mu_\pi^2}{M^2} + \frac{60}{51}l_{12} - \frac{9}{51}l_3 + \frac{49}{51} \\ T_F &= \ln \frac{\mu_\pi^2}{M^2} + l_{12} + \frac{1}{5}(l_3 - l_4) + \frac{23}{30}. \end{aligned} \quad (11)$$

Our analysis convention is to fix $a_M = -1/2$ and $a_F = 1$ in any fit. Then at NLO there are four LEC's which can be measured, B , F , l_3 and l_4 . NNLO adds an additional three LEC's, (l_{12}, k_M, k_F) to the collection of quantities to be fit. The LEC's are expected to show the following N_c scaling (the quick list can be found in Ref. [18]):

$$O(N_c): F^2, L_5, L_8, \quad O(1): B, L_4, L_6. \quad (12)$$

This means that the l_i 's for $i = 3, 4$ scale as

$$l_i = N_c l_i^{(0)} + l_i^{(1)}. \quad (13)$$

Our analysis of data using $SU(N_f)$ chiral perturbation theory is done with separate fits for each N_c . We can then ask whether the LEC's scale with N_c as given by Eqs. (12)–(13).

The “ ξ -convention” rewrites the chiral expansion in terms of a ratio of observables

$$\xi = \frac{m_{\text{PS}}^2}{8\pi^2 f_{\text{PS}}^2} \quad (14)$$

(in the “132 MeV” definition for the decay constant). We have only implemented the NLO expressions, which are

$$M^2 = 2Bm_q = m_{\text{PS}}^2 \left[1 + \frac{1}{2} \xi \left(\ln \frac{\mu^2}{m_{\text{PS}}^2} + l_3 \right) \dots \right] \quad (15)$$

and

$$F = f_{\text{PS}} \left[1 - \xi \left(\ln \frac{\mu^2}{m_{\text{PS}}^2} + l_4 \right) + \dots \right]. \quad (16)$$

The ξ parametrization is often used because the coefficients of higher order terms [here order (ξ^2)] are smaller than in the x parametrization. It is more awkward to use in a fit since the expressions have to be inverted (to express measured quantities such as $f_{\text{PS}} \pm \Delta f_{\text{PS}}$ in terms of fit parameters). At NLO, the relevant expressions are

$$\begin{aligned} f_{\text{PS}} &= \frac{F}{2} \left[1 + \left(1 + 4 \frac{m_{\text{PS}}^2}{8\pi^2 F^2} \left(\ln \frac{\mu^2}{m_{\text{PS}}^2} + l_4 \right) \right)^{1/2} \right] \\ &\equiv \mathcal{F}(F, l_4, m_{\text{PS}}^2). \end{aligned} \quad (17)$$

and

$$m_q = \frac{m_{\text{PS}}^2}{2B} \left[1 + \frac{1}{2} \left(\frac{m_{\text{PS}}^2}{8\pi^2 \mathcal{F}(F, l_4, m_{\text{PS}}^2)} \right) \left(\log \frac{\mu^2}{m_{\text{PS}}^2} + l_3 \right) \right]. \quad (18)$$

The $U(N_f)$ chiral Lagrangian includes the eta prime in its degrees of freedom. The appropriate effective field theory was developed in Refs. [10–15]. The power counting is

$$O(\delta) \sim O(p^2) \sim O(M^2) \sim O(m_q) \sim (1/N_c) \quad (19)$$

(Notice that $1/F^2$ is $O(\delta)$ and the $SU(N_f)$ chiral expansion parameter x of Eq. (4) is $O(\delta^2)$.)

For f_{PS} and m_{PS}^2 the many LEC's of the complete theory reduce to two, each with its own expansion in N_c , as given by Eq. (13) as in the $SU(N_f)$ case. The factors of N_c in the various l_i 's of the $SU(N_f)$ expressions give $O(1/\delta)$ scaling factors in the $U(N_f)$ perturbative expansion. Thus, all that survives from the x^2 terms T_M and T_F in Eq. (11) are constants proportional to N_c^2 .

The eta prime enters as an additional Nambu-Goldstone boson of the nonanomalous (in the large N_c limit) singlet $U(1)_A$ symmetry. It appears in the perturbative expansion as an extra tadpole contribution. The perturbative calculations for f_{PS} and m_{PS}^2 can be found in Ref. [21], are succinctly presented for the degenerate-flavor case in Ref. [18], and can be reassembled (if desired) by slightly editing the calculation of Ref. [22].

The formulas for the chiral expansion need the mass of the eta prime and its decay constant as a function of N_c . The calculation of the eta prime mass for $N_c = 3$ is already a difficult problem (the statistics of a recent study [23] dwarf

those of our little project) and so we have recourse to theory. Witten and Veneziano [24,25] related the eta prime mass to the quenched topological susceptibility χ_T and the pseudoscalar decay constant F (recall the 132 MeV convention),

$$M_{\eta'}^2 = M^2 + M_0^2 \quad (20)$$

where the zero-quark mass eta prime mass is

$$M_0^2 = \frac{4N_f \chi_T}{F^2}. \quad (21)$$

Note that M_0^2 is also $O(\delta)$. There is indirect lattice evidence in favor of this relation from the study of the $N_f = 2$ topological susceptibility across N_c from Ref. [26]. A phenomenological formula which relates the quenched topological susceptibility to the topological susceptibility at small quark mass due to Refs. [10,27,28] agreed qualitatively with lattice results.

We thus proceed, taking Eq. (20) for the eta prime mass, assuming that the eta prime and the pions share a common decay constant, and defining

$$\begin{aligned} x_{\eta'} &= \frac{M_{\eta'}^2}{8\pi^2 F^2} \\ x_0 &= \frac{M_0^2}{8\pi^2 F^2} \end{aligned} \quad (22)$$

to write

$$\begin{aligned} m_{\text{PS}}^2 &= M_{\text{NLO}}^2 + M_{\text{NNLO}}^2 \\ f_{\text{PS}} &= F_{\text{NLO}} + F_{\text{NNLO}} \end{aligned} \quad (23)$$

where

$$\begin{aligned} M_{\text{NLO}}^2 &= 2Bm_q \left[1 - \frac{x}{2} N_c l_3^{(0)} \right] \\ F_{\text{NLO}} &= F \left[1 + x N_c l_4^{(0)} \right] \end{aligned} \quad (24)$$

and

$$\begin{aligned} M_{\text{NNLO}}^2 &= 2Bm_q \left[-\frac{x}{2} \left(\log \frac{\mu^2}{M^2} + l_3^{(1)} \right) + \frac{x_{\eta'}}{2} \log \frac{\mu^2}{M_{\eta'}^2} \right. \\ &\quad \left. + x^2 N_c^2 T_M \right] \\ F_{\text{NNLO}} &= F \left[x \left(\log \frac{\mu^2}{M^2} + l_4^{(1)} \right) + x^2 N_c^2 T_F \right]. \end{aligned} \quad (25)$$

We use Eqs. (23)–(25) for fits to the data at an individual N_c value. Notice that, in that case, the NLO fits give $l_i^{(0)}$, but the NNLO fits can only give the full $l_i = N_c l_i^{(0)} + l_i^{(1)}$.

We can present results for the LEC's as we do for the $SU(N_f)$ case, a plot of, for example, F versus $1/N_c$.

We can also imagine doing combined fits to the data. In that case we would make an ansatz, that

$$\begin{aligned} F &= \sqrt{\frac{N_c}{3}} \left(f_0 + \frac{f_1}{N_c} + \frac{f_2}{N_c^2} \right) \\ B &= b_0 + \frac{b_1}{N_c} + \frac{b_2}{N_c^2}. \end{aligned} \quad (26)$$

We would insert these expressions in Eqs. (24)–(25), combine them systematically along with the other LEC's, and fit a range of N_c values. In order to do this, of course, the $U(N_f)$ chiral expansion has to be well behaved for all the individual N_c values included in the fit. We return to this point when we present fit results in Sec. V, but for now we remark that our $N_c = 3$ data is incompatible with the $U(2)$ expansion leaving only two N_c 's to work with; too few values of N_c to think about NNLO fits. So we did not pursue this line.

We note that the LEC's of $SU(N_f)$ chiral perturbation theory and $U(N_f)$ chiral perturbation theory are not identical [15,29]. In particular, there are shifts

$$\begin{aligned} B(SU(N_f)) &= B(U(N_f)) \left[1 + \frac{1}{N_f} x_0 \log \frac{\mu^2}{M_0^2} \right] \\ L_3^{(1)}(SU(N_f)) &= L_3^{(1)}(U(N_f)) + \log \frac{\mu^2}{M_0^2} - 1. \end{aligned} \quad (27)$$

The shift in the B 's is formally order $1/N_c^2$ but the prefactor happens to be large. Note also that, in contrast to the $SU(N_f)$ case, in the $U(N_f)$ expansion a shift in the regularization point μ affects the value of B . FLAG [16] quotes values for the LEC's using μ^2 set to the physical squared pion mass. This choice causes a large shift between the NLO and NNLO determinations of B at low N_c . To avoid this large logarithm, we choose a regularization point closer to the eta prime mass; we take μ^2 to be an N_c -independent quantity which we choose to be $\mu^2 = 8\pi^2 f_\pi^2$ where $f_\pi = 132$ MeV in all our comparison of lattice data to the $U(N_f)$ expansion. When we compare the $U(2)$ LEC's to the $SU(2)$ ones, there will also be a shift in the $SU(2)$ l_i 's due to the different choices for μ , see Eq. (8).

III. DETAILS OF THE NUMERICAL SIMULATIONS

The project involves simulations at three values of N_c . Each N_c value requires its own set of simulations at four bare gauge couplings and 4-6 bare quark masses per gauge coupling. At each bare parameter value six quantities are measured: the axial Ward identity fermion mass, the pseudoscalar mass, the pseudoscalar decay constant, two lattice to continuum renormalization factors (for the fermion mass and decay constant), as well as a parameter to set the lattice spacing. All these quantities must be checked

for correlations. The lattice regulated quantities are converted into dimensionless continuum regulated quantities which are then fit to the formulas described in the last section, plus lattice artifacts. Doing this is a long and somewhat recursive task. We believe that the methodology we use to generate, collect, and analyze our lattice datasets is completely standard. However, all lattice calculations involve many choices. This section describes what we did in perhaps too much detail.

A. Simulation details: Lattice action, updating algorithm, datasets, observables

Our simulations are done with the usual Wilson plaquette action, with the bare gauge coupling g_0 labeled by $\beta = 2N_c/g_0^2$. Two flavors of degenerate mass fermions (discretized as Wilson-clover fermions) are included. Configurations are generated using the hybrid Monte Carlo (HMC) algorithm [30–32] with a multilevel Omelyan integrator [33] and multiple integration time steps [34] with one level of mass preconditioning for the fermions [35].

The fermion action uses gauge connections defined as normalized hypercubic (nHYP) smeared links [36–38]. Simulations use the arbitrary N_c implementation of Ref. [39]. The bare quark mass m_0^q appears in the lattice action along with the lattice spacing a via the hopping parameter $\kappa = (2m_0^q a + 8)^{-1}$. The clover coefficient is fixed to its tree level value, $c_{\text{SW}} = 1$. The gauge fields obey periodic boundary conditions; the fermions are periodic in space and antiperiodic in time.

Lattice volumes are a mix of $16^3 \times 32$ and $24^3 \times 32$ sites. The lattice sizes were chosen so as to minimize finite volume effects (which we describe in Sec. III C below). Briefly, we began simulation runs at nearly all our bare parameter values taking 16^3 spatial volumes and collected enough data to determine the mass and decay constant of a pseudoscalar meson, and then to estimate the size of the finite volume correction. When this appeared to be larger than a few per cent, we replaced the 16^3 datasets by 24^3 ones. A glance at Tables I–III shows that there are more 24^3 $N_c = 3$ datasets than there are for $N_c = 4$ or 5. This is because of the scaling of the pseudoscalar decay constant with N_c , as described in the Introduction.

Lattices used for analysis are spaced a minimum of 10 HMC time units apart, so individual bare parameter sets contain 30 to 200 stored lattices. All datasets at individual bare parameters (β, κ) are based on a single stream. We check for thermalization at the start of each data stream (which typically begins from an equilibrated configuration at a nearby bare parameter set) and typically discard the first 100 trajectories (more than this for simulations at strong coupling). The datasets are extensions of ones presented in Refs. [39,40].

Data for the pseudoscalar mass, the pseudoscalar decay constant, and the fermion mass come from hadron correlators

TABLE I. Lattice data for $N_c = 3$. The entries C_1 , C_2 , and C_3 correspond to the correlation coefficients $C_{m_q, m_{\text{PS}}}$, $C_{m_q, f_{\text{PS}}}$, and $C_{m_{\text{PS}}, f_{\text{PS}}}$.

κ	L	am_q	am_{PS}	af_{PS}	t_0/a^2	C_1	C_2	C_3	Z_A	Z_m	N_{conf}
$\beta = 5.25$											
0.1284	16	0.0628(5)	0.4743(31)	0.519(28)	0.927(3)	0.423	0.196	-0.120	0.984(11)	1.011(37)	50
0.1288	16	0.0476(6)	0.4135(34)	0.4937(80)	0.981(3)	0.508	0.438	0.314	0.962(8)	1.010(40)	90
0.1292	16	0.0324(5)	0.3371(27)	0.4479(64)	1.045(3)	0.564	0.417	0.106	0.955(7)	1.024(37)	90
0.1294	16	0.0253(5)	0.2926(36)	0.4234(90)	1.076(4)	0.546	0.567	0.280	0.967(8)	1.033(42)	90
0.1296	16	0.0189(4)	0.2488(36)	0.443(13)	1.128(7)	0.393	0.608	0.093	0.946(7)	1.064(30)	90
$\beta = 5.3$											
0.1280	16	0.0470(4)	0.3956(24)	0.438(17)	1.249(10)	0.034	0.466	-0.073	0.978(10)	1.026(34)	90
0.1284	16	0.0334(3)	0.3213(36)	0.3969(59)	1.326(5)	0.251	0.583	0.216	0.980(14)	1.033(31)	110
0.1285	16	0.0288(13)	0.3022(31)	0.3961(74)	1.381(5)	0.454	0.407	0.211	0.961(9)	1.038(30)	90
0.1286	16	0.0244(3)	0.263(15)	0.3705(87)	1.414(6)	-0.006	-0.112	0.065	0.966(8)	1.071(24)	90
0.1288	24	0.0177(3)	0.2333(44)	0.3580(64)	1.449(5)	0.310	0.457	0.113	0.959(6)	0.999(35)	73
$\beta = 5.35$											
0.1270	16	0.0581(4)	0.4124(66)	0.429(22)	1.557(10)	0.011	0.510	0.073	0.989(10)	1.021(30)	30
0.1275	16	0.0396(4)	0.3361(41)	0.368(16)	1.729(10)	0.268	0.112	0.435	0.986(7)	1.046(27)	50
0.12775	16	0.0322(3)	0.3115(49)	0.376(12)	1.742(7)	0.110	0.452	0.179	0.983(8)	1.041(26)	110
0.1280	24	0.0237(4)	0.2556(37)	0.3485(60)	1.831(8)	0.671	0.388	-0.079	0.969(6)	1.037(25)	150
0.1282	24	0.0169(2)	0.2224(17)	0.326(14)	1.888(5)	0.443	0.351	0.115	0.962(6)	1.059(23)	90
0.1283	24	0.0132(2)	0.1916(28)	0.3216(73)	1.937(8)	0.339	0.396	-0.096	0.962(6)	1.085(20)	89
0.1284	24	0.0097(2)	0.1650(66)	0.2988(68)	1.982(6)	-0.116	0.410	-0.243	0.956(7)	1.072(24)	90
$\beta = 5.4$											
0.1265	24	0.0565(9)	0.3889(16)	0.399(13)	2.028(9)	-0.046	0.081	-0.194	0.989(9)	1.032(27)	90
0.1270	24	0.0410(2)	0.3282(14)	0.3631(77)	2.155(7)	0.291	0.161	-0.271	0.984(8)	1.055(22)	90
0.1272	24	0.0339(2)	0.2976(25)	0.3463(35)	2.240(8)	0.227	0.217	0.299	0.974(7)	1.058(25)	90
0.1276	24	0.0203(6)	0.2360(59)	0.3050(30)	2.372(8)	-0.157	0.002	0.015	0.973(6)	1.076(20)	90
0.1277	24	0.0169(2)	0.2102(20)	0.2977(77)	2.430(10)	0.188	0.489	-0.208	0.971(8)	1.046(26)	90
0.1278	24	0.0138(3)	0.1855(21)	0.2836(58)	2.467(10)	0.402	0.032	-0.075	0.967(6)	1.063(24)	90
0.1279	24	0.0104(2)	0.1631(58)	0.2754(91)	2.574(13)	0.218	0.696	0.172	0.970(6)	1.112(18)	90

using propagators constructed in Coulomb gauge, with Gaussian sources and $\vec{p} = 0$ point sinks. We tune the width of the source to minimize the dependence of the effective mass [defined, as usual, to be $m_{\text{eff}}(t) = \log C(t)/C(t+1)$ in the case of open boundary conditions for the correlator $C(t)$] on the distance t between source and sink. All results are based on a standard full correlated analysis involving fits to a wide range of t 's. Best fits are chosen with the ‘‘model averaging’’ ansatz of Jay and Neil [41]. In one sentence, this gives each particular fit in a suite (with a chi-squared value χ^2 and N_{DOF} degrees of freedom) a weight in the average which is proportional to $\exp(-(\chi^2/2 - N_{\text{DOF}}))$.

The pseudoscalar decay constant is defined in terms of the matrix element of the timelike component of the axial current $A_0(x, t) = \bar{u}(x, t)\gamma_0\gamma_5 d(x, t)$ between the vacuum and a pseudoscalar state as in Eq. (3). It is determined via a correlated fit to two propagators with a common source,

$$\begin{aligned}
C_1(t) &= \sum_{\mathbf{x}} \langle A_0(\mathbf{x}, t) \mathcal{O}(0, 0) \rangle \\
C_2(t) &= \sum_{\mathbf{x}} \langle \mathcal{O}(\mathbf{x}, t) \mathcal{O}(0, 0) \rangle.
\end{aligned} \tag{28}$$

The fermion mass am_q is taken to be the axial Ward identity (AWI) fermion mass, defined through the relation of the axial current matrix element to the pseudoscalar $P(x, t) = \bar{u}(x, t)\gamma_5 d(x, t)$,

$$\partial_t \sum_{\mathbf{x}} \langle A_0(\mathbf{x}, t) \mathcal{O} \rangle = 2am_q \sum_{\mathbf{x}} \langle P^a(\mathbf{x}, t) \mathcal{O} \rangle, \tag{29}$$

again taken from a simultaneous fit to two two-point functions. \mathcal{O} can be any convenient source, of course, and for us it is a Gaussian.

Conversion factors from lattice regulated quantities will be needed for f_{PS} and m_q and their calculation will be described in Sec. III D below.

The pseudoscalar mass am_{PS} is determined from fits involving correlators of pseudoscalar currents.

We give a brief summary of the datasets. We attempted to collect data at similar values of $\xi = m_{\text{PS}}^2/(8\pi^2 f_{\text{PS}}^2)$ for our different values of N_c , since that is the expansion parameter for chiral perturbation theory.

For $N_c = 3$ we have four beta values and 24 bare parameter sets in total. The ξ range is from 0.06 to 0.19. $t_0 m_{\text{PS}}^2$ ranges from 0.05 to 0.35, for pion masses in the range 300–776 MeV (taking a nominal value for the flow

TABLE II. Lattice data for $N_c = 4$. The entries C_1 , C_2 , and C_3 correspond to the correlation coefficients $C_{m_q, m_{\text{PS}}}$, $C_{m_q, f_{\text{PS}}}$, and $C_{m_{\text{PS}}, f_{\text{PS}}}$.

κ	L	am_q	am_{PS}	af_{PS}	t_0/a^2	C_1	C_2	C_3	Z_A	Z_m	N_{conf}
$\beta = 10.0$											
0.1270	16	0.1017(4)	0.6159(15)	0.7086(77)	0.855(2)	0.603	0.419	0.261	0.992(15)	0.994(44)	61
0.1280	16	0.0570(10)	0.4461(45)	0.610(21)	1.023(4)	0.620	0.187	0.258	0.984(14)	1.011(41)	40
0.1285	16	0.0359(4)	0.3456(22)	0.5262(87)	1.131(5)	0.522	0.018	-0.207	0.974(10)	1.038(36)	50
0.1288	16	0.0240(6)	0.2798(44)	0.483(14)	1.194(6)	0.472	0.528	0.357	0.973(11)	1.072(31)	90
0.1289	16	0.0192(4)	0.2504(34)	0.482(12)	1.230(7)	0.421	0.636	0.284	0.974(12)	1.053(33)	90
0.1290	16	0.0158(3)	0.2264(29)	0.489(14)	1.241(6)	0.396	0.490	-0.130	0.963(6)	1.102(25)	80
$\beta = 10.1$											
0.1250	16	0.1161(1)	0.6168(15)	0.6138(96)	1.321(6)	0.275	0.329	0.180	1.020(13)	0.978(38)	90
0.1266	16	0.0623(2)	0.4324(16)	0.5255(71)	1.565(7)	0.547	0.200	0.188	0.998(10)	1.025(28)	80
0.1270	16	0.0481(2)	0.3743(35)	0.4905(52)	1.665(8)	0.273	0.214	0.321	0.999(8)	1.033(26)	80
0.1275	16	0.0311(2)	0.2988(18)	0.4391(97)	1.772(11)	0.361	-0.001	0.306	0.987(12)	1.050(27)	90
0.12765	16	0.0264(1)	0.2740(14)	0.4420(41)	1.786(7)	0.381	0.227	-0.028	0.975(7)	1.056(24)	140
0.12775	16	0.0226(2)	0.2556(15)	0.4132(76)	1.831(9)	0.387	-0.140	-0.182	0.988(10)	1.038(31)	120
0.1280	16	0.0147(5)	0.2017(56)	0.3955(78)	1.883(13)	0.757	-0.035	-0.185	0.977(8)	1.083(22)	50
$\beta = 10.2$											
0.1252	16	0.0866(2)	0.4897(22)	0.4957(28)	2.080(3)	0.645	0.333	0.418	1.012(9)	1.005(30)	190
0.1262	16	0.0547(1)	0.3783(15)	0.4473(35)	2.270(4)	0.185	0.356	0.328	1.002(8)	1.036(23)	190
0.1265	16	0.0454(2)	0.3415(16)	0.4314(50)	2.312(10)	0.088	0.315	-0.158	0.992(6)	1.045(22)	90
0.1270	16	0.0290(2)	0.2709(19)	0.3881(44)	2.452(5)	0.136	0.188	-0.045	0.982(5)	1.079(20)	101
0.1272	16	0.0222(1)	0.2387(36)	0.3659(97)	2.520(20)	0.041	0.210	-0.186	0.983(7)	1.079(20)	90
0.1273	16	0.0191(2)	0.2229(36)	0.3555(94)	2.543(17)	0.293	0.281	-0.288	0.983(8)	1.085(18)	90
0.1275	24	0.0124(1)	0.1760(12)	0.3429(41)	2.621(9)	0.295	0.401	-0.241	0.980(7)	1.090(18)	90
$\beta = 10.3$											
0.1260	16	0.0494(3)	0.3391(40)	0.3910(62)	3.106(17)	0.689	0.489	0.494	0.997(8)	1.046(22)	50
0.1265	16	0.0337(1)	0.2826(23)	0.3503(53)	3.139(14)	0.160	0.129	-0.141	0.990(7)	1.080(17)	98
0.12675	16	0.0255(1)	0.2454(23)	0.3347(49)	3.277(28)	0.208	0.420	-0.110	0.989(6)	1.067(16)	90
0.1270	16	0.0174(1)	0.2020(35)	0.3124(85)	3.375(21)	0.271	-0.057	-0.212	0.982(6)	1.084(10)	90
0.1271	24	0.0142(1)	0.1791(21)	0.3044(34)	3.436(13)	0.408	-0.072	-0.464	0.979(4)	1.094(16)	90
0.1272	24	0.0108(1)	0.1595(26)	0.2918(35)	3.514(14)	-0.282	0.148	-0.015	0.978(7)	1.079(20)	90

parameter $\sqrt{t_0} = 0.15$ fm from Ref. [42]). t_0/a^2 ranges from 1.0 to 2.4 for lattice spacings between 0.10–0.15 fm.

The $N_c = 4$ datasets come from four beta values and there are 26 bare parameter sets. ξ ranges from 0.04 to 0.2 and $t_0 m_{\text{PS}}^2$ is in the range 0.06–0.67. t_0/a^2 is in the range 1.1–3.34 for $a = 0.08$ –0.14 fm.

And there are four beta values and 21 bare parameter sets in the $N_c = 5$ sector. ξ ranges from 0.05 to 0.16, $t_0 m_{\text{PS}}^2$ is in the range 0.10–0.63, while t_0 lies between 1.5 and 3.4, or $a = 0.08$ –0.12 fm.

A useful marker point is $\xi = 0.1$, for which $t_0 m_{\text{PS}}^2$ is about 0.10, 0.22, and 0.35 for $N_c = 3, 4$, or 5. This quantity will reappear in Sec. V.

Another marker is a comparison with the large N_c study of Ref. [18]. Their datasets were collected at fixed fermion masses across N_c and spanned $\xi \in (0.10 - 0.16)$ for $N_c = 3$, $\xi \in (0.05 - 0.09)$ for $N_c = 4$, $\xi \in (0.04 - 0.08)$ for $N_c = 5$, and $\xi \in (0.03 - 0.06)$ for $N_c = 6$. The lower part of our ξ ranges overlap with theirs.

The data are presented in Tables I–III.

B. Setting a scale

The conversion of simulations quantities whose scale is set by the lattice spacing into dimensionless parameters which can be used in continuum extrapolations is done using the Wilson flow parameter t_0 [8,9]. The determination of t_0 from each dataset (with its own β and κ) is done in the standard way, from the observable $E(t_0)$ extracted from the field strength tensor,

$$t_0^2 \langle E(t_0) \rangle = C(N_c). \quad (30)$$

$C(N_c)$ is chosen to match what most other large N_c simulations take,

$$C(N_c) = \frac{3}{8} \left(\frac{N_c^2 - 1}{N_c} \right) \times C \quad (31)$$

with $C = 0.3$ the usual value used in $SU(3)$. The motivation for this choice is that $C(N_c)$ should be rescaled proportionally to the quadratic Casimir of the fundamental

TABLE III. Lattice data for $N_c = 5$. The entries C_1 , C_2 , and C_3 correspond to the correlation coefficients $C_{m_q, m_{\text{PS}}}$, $C_{m_q, f_{\text{PS}}}$, and $C_{m_{\text{PS}}, f_{\text{PS}}}$.

κ	L	am_q	am_{PS}	af_{PS}	t_0/a^2	C_1	C_2	C_3	Z_A	Z_m	N_{conf}
$\beta = 16.2$											
0.1250	16	0.1218(4)	0.6461(23)	0.7055(92)	1.161(4)	0.421	0.448	0.507	1.029(16)	0.950(44)	60
0.1260	16	0.0871(4)	0.5309(20)	0.6650(61)	1.290(7)	0.545	0.426	0.083	1.020(14)	0.988(38)	30
0.1270	16	0.0517(4)	0.4011(22)	0.599(15)	1.451(21)	0.247	-0.000	0.572	0.997(12)	1.033(30)	30
0.1278	16	0.0249(2)	0.2708(19)	0.5250(65)	1.562(10)	0.427	0.502	0.018	0.987(9)	1.058(28)	70
$\beta = 16.3$											
0.1250	16	0.0982(3)	0.5383(27)	0.612(18)	1.709(7)	0.414	-0.087	-0.027	1.033(12)	0.979(33)	50
0.1260	16	0.0667(2)	0.4377(17)	0.5700(73)	1.823(6)	-0.205	-0.035	0.243	1.007(11)	1.015(28)	50
0.1264	16	0.0543(1)	0.3880(13)	0.554(18)	1.871(7)	0.375	0.227	-0.112	1.010(11)	1.031(25)	90
0.1268	16	0.0409(3)	0.3335(12)	0.514(14)	1.940(11)	0.118	0.615	0.071	0.995(11)	1.045(23)	90
0.1270	16	0.0346(1)	0.3070(17)	0.4992(51)	1.950(8)	-0.033	0.336	-0.199	0.996(9)	1.056(24)	90
0.1273	16	0.0249(1)	0.2551(12)	0.4795(49)	2.030(8)	0.079	0.243	-0.065	0.996(8)	1.060(22)	110
0.1275	16	0.0183(2)	0.2220(23)	0.4444(68)	2.057(7)	0.299	0.141	-0.004	0.986(7)	1.066(21)	50
$\beta = 16.4$											
0.1252	16	0.0818(1)	0.4701(7)	0.5510(25)	2.181(4)	0.167	0.183	0.160	1.015(11)	1.006(28)	190
0.1258	16	0.0631(1)	0.4037(14)	0.5194(42)	2.272(5)	-0.161	0.104	0.023	1.008(10)	1.019(24)	190
0.1265	16	0.0409(1)	0.3228(11)	0.4792(55)	2.386(6)	0.206	0.351	0.242	1.000(11)	1.047(23)	190
0.1270	16	0.0247(1)	0.2478(16)	0.4283(25)	2.483(6)	0.161	0.114	-0.146	0.986(9)	1.081(18)	200
0.1272	24	0.0183(1)	0.2122(8)	0.4236(68)	2.526(6)	0.070	0.074	-0.128	0.987(10)	1.082(19)	90
$\beta = 16.6$											
0.1252	16	0.0695(1)	0.4040(12)	0.4705(37)	3.136(12)	0.255	0.292	0.063	1.020(11)	1.024(24)	90
0.1260	16	0.0443(1)	0.3186(15)	0.4171(45)	3.360(22)	0.164	0.102	0.197	1.005(7)	1.051(21)	110
0.1264	16	0.0318(1)	0.2674(15)	0.3934(37)	3.407(22)	0.253	0.037	0.029	0.993(4)	1.067(18)	140
0.1266	16	0.0254(1)	0.2382(22)	0.3712(63)	3.455(16)	-0.243	-0.133	0.060	1.002(9)	1.078(16)	140
0.1269	24	0.0159(0)	0.1814(12)	0.3591(31)	3.543(12)	0.281	0.257	-0.282	0.988(7)	1.093(16)	90

representation of the gauge group. Our procedure for computing t_0 from the data is identical to what was done in Ref. [26] and details may be found there.

In contrast to our earlier work, where conversion from dimensional to dimensionless parameter $[(am_{\text{PS}})^2$ to $t_0 m_{\text{PS}}^2$, for example] was done at individual bare parameter values with a $t_0(\beta, \kappa)$, we need to use a mass-independent definition of t_0 . This is because the chiral expansion for t_0 has its own set of NLO analytic contributions which combine with the ones for our desired observables (f_{PS} and m_{PS}^2) [43] and would contaminate the chiral LEC's. We also need a scale choice which is superficially identical across N_c .

We investigated several possibilities

- (i) t_0 at a fixed value $(N_c/3)\xi$ —This is a bit awkward to produce, since it needs Z_A , the axial current matching factor.
- (ii) t_0 at fixed m_{PS}^2/m_V^2 (where m_V is the mass of the vector meson)—This was noisier than the first choice.
- (iii) t_0 at fixed $t_0 m_{\text{PS}}^2$ —This was also noisier than the first choice (and with greater correlations).

We arbitrarily selected the first choice, $(N_c/3)\xi \equiv \xi_0$.

Then we followed the following procedure to produce a value of t_0 at each β value. Each dataset gives its own $\xi_0 \pm \Delta\xi_0$ and $t_0 \pm \Delta t_0$. For each β value, we performed a

polynomial fit $t_0(i) = \sum_n C_n (\xi(i) - \xi_0)^n$ to produce a value of $t_0(\xi_0, \beta)$. The fit included the errors Δt_0 and $\Delta\xi$. (See Sec. IV for a discussion about fit methodology.) We checked subsets of the data to see if correlations in t_0 and ξ affected the fit. They did not (differences in correlated and uncorrelated fits for $t_0(\xi_0)$ were well under a standard deviation) so we did not include them in our analysis. We typically fit to a cubic, bracketing ξ_0 so that the fit was essentially an interpolation.

Our choice of ξ_0 is purely heuristic. We have to make sure ξ_0 lies inside the range of measured $(N_c/3)\xi$ values recorded for each bare parameter set, and then we simply pick a ξ_0 for which Δt_0 is minimized. Like many other decisions made in the data analysis, we looked at many possible choices but we saw little effect on results. In the end, we took $\xi_0 = 0.12$.

An example of the extraction of t_0 from data, for $N_c = 5$, is shown in Fig. 1, and the data are collected in Table IV.

C. Correcting for finite volume

Our smallest quark mass data could potentially be affected by our simulation volumes. For chiral observables, the cause is well known: tadpole graphs, where a pseudo-scalar particle is emitted from some location and returns to the same point, are replaced by a set of contributions connecting the location to its image points. (We found the

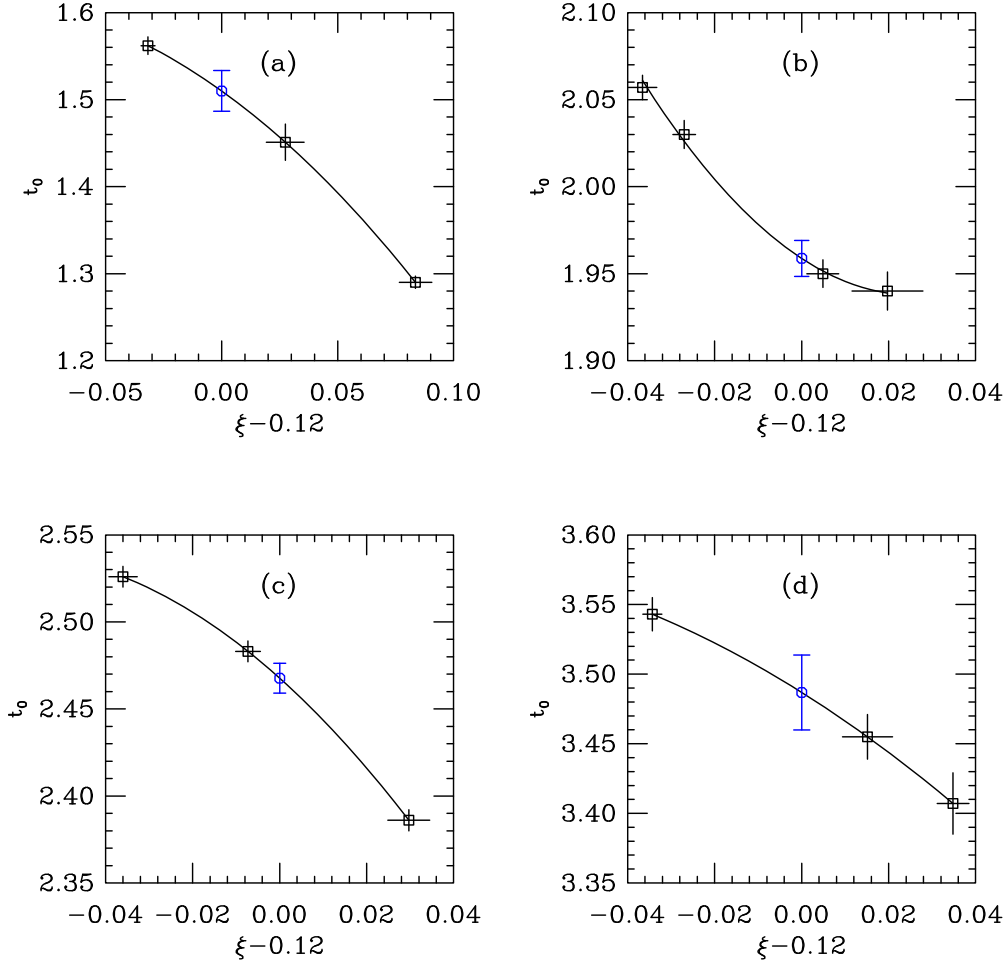


FIG. 1. Interpolating to find a fiducial t_0 , for $N_c = 5$ datasets. The data at individual κ values are shown in squares; the interpolated value is an octagon (in blue). Panels are (a) $\beta = 16.2$, (b) $\beta = 16.3$, (c) $\beta = 16.4$ (d) $\beta = 16.6$.

discussion in Ref. [44] to be quite helpful.) If we write the pseudoscalar correlator for a particle of mass m in a box of length L_μ in direction μ as

$$\Delta(m, x) \rightarrow \sum_{n_\mu} \Delta(m, x + n_\mu L_\mu), \quad (32)$$

the infinite volume propagator, call it $\bar{\Delta}(m, x)$, is the $n = 0$ term in the sum. The finite volume tadpole is

$$\Delta(m, 0) = \bar{\Delta}(m, 0) + \bar{I}_1(m, L) \quad (33)$$

where $\bar{I}_1(m, L)$ is the sum over images. If a typical infinite volume observable has a chiral expansion

$$O(L = \infty) = O_0 \left[1 + C_0 \frac{1}{f_{\text{PS}}^2} \bar{\Delta}(m, 0) \right] \quad (34)$$

then the finite volume correction is

$$O(L) - O(L = \infty) = O_0 \left[C_0 \frac{1}{f_{\text{PS}}^2} \bar{I}_1(m, L) \right]. \quad (35)$$

We replace the simulation observable in our dataset $O(L)$ by

$$O(L = \infty) = \frac{O(L)}{1 + C_0 \frac{1}{f_{\text{PS}}^2} \bar{I}_1(m, L)}. \quad (36)$$

$\bar{I}_1(m, L)$ can be found from

$$\begin{aligned} \Delta(x) &= \int \frac{d^4 p}{(2\pi)^4} \frac{\exp(ipx)}{p^2 + m^2} \\ &= \frac{m}{16\pi^2 x} \int_0^\infty dk \exp\left(-mx \left(\frac{k}{4} + \frac{1}{k}\right)\right) \end{aligned} \quad (37)$$

by summing over all image points until the expression saturates.

Equation (36) also needs f_{PS} , the decay constant in the chiral limit. This is, of course a parameter in the fit.

TABLE IV. Flow parameter values at $\xi_0 = 0.12$.

β	t_0/a^2
<i>SU(3)</i>	
5.25	1.037(7)
5.3	1.374(13)
5.35	1.804(17)
5.4	2.379(19)
<i>SU(4)</i>	
10.0	1.116(14)
10.1	1.770(12)
10.2	2.503(33)
10.3	3.339(25)
<i>SU(5)</i>	
16.2	1.510(23)
16.3	1.959(10)
16.4	2.468(8)
16.6	3.487(27)

However, if we just make an estimate for it and evaluate Eq. (36), we find that for all our datasets, the correction is at most on the order of a few per cent for a few of the lightest-mass points, so we only need to input an approximate value of f_{PS} given all the other uncertainties in the calculation. We use $\sqrt{t_0}f_{\text{PS}} = 0.078, 0.107, 0.128$ for $N_c = 3, 4, 5$.

D. Lattice to continuum regularization conversion

We will use the ‘‘regularization independent’’ or RI scheme [45] for computing matching factors (labeled as Z_i for current i). The method is standard and so we will only briefly describe our particular implementation of it.

One computes quark and gluon Green’s functions in Landau gauge, regulated by giving all external lines a large Euclidean squared momentum $p^2 = \mu^2$, and uses combinations of them to determine the Z ’s. Specifically, we define

$$\mu^2 = \sum_i 4 \sin^2 \frac{p_i}{2} + 4 \sin^2 \frac{p_t}{2} \quad (38)$$

where $p_i = 2n_i\pi/L$ and $p_t = (2n_t + 1)\pi/T$ since the temporal boundary conditions are anti-periodic. (Recall that the lattices are $L^3 \times T$ sites.)

The matching factor is defined by computing the ratio of the matrix elements of the operator between off-shell single particle momentum eigenstates in the full and free theories

$$Z_{\Gamma}^{RI}(\mu) \langle p | O_{\Gamma} | p \rangle_{p^2=\mu^2} = \langle p | O_{\Gamma} | p \rangle_0. \quad (39)$$

or equivalently

$$Z_{\Gamma}^{RI}(\mu) \frac{1}{4N_c} \text{Tr}[\langle p | O_{\Gamma} | p \rangle_{p^2=\mu^2} \langle p | O_{\Gamma} | p \rangle_0^{-1}] = 1, \quad (40)$$

where the factor of $1/4N_c$ counts Dirac spins and colors. We use the RI' scheme to define Z_Q from a projection against the free propagator $S_0(p)$:

$$Z_Q^{RI'} = \frac{1}{4N_c} \text{Tr}S(p)S_0^{-1}(p). \quad (41)$$

We are using clover fermions, for which there is an overall 2κ factor in the field definition as opposed to a continuum like normalization. We define our Z_{Γ} factors for observables built from clover fermions by

$$\langle h | \Gamma | h' \rangle_{\text{cont}} = \langle h | \Gamma | h' \rangle_{\text{latt}} \times 2\kappa Z_{\Gamma} \quad (42)$$

where $Z_{\Gamma} \sim 1 + Cg^2 \dots$ in a perturbative expansion. The 2κ factor gives clover Z ’s equal to unity for free field theory.

One needs the scale μ to be large enough not to be affected by confinement effects but not so large that is affected by lattice artifacts. Given our lattice spacings and volumes, this means in practice a value of μa around unity.

We need a renormalization factor for the axial current, Z_A , to define F and one for the fermion mass Z_m to carry the quark mass to a continuum regularization. The computations are straightforward. We generate lattice data for $Z_A(a\mu)$ at many values of $(a\mu)^2 = \sum_j a^2 p_j^2$ for lattice momenta ap_j . The data is averaged under single elimination jackknife and sorted in $a\mu$. Fits to a linear function are performed over ‘‘windows’’ of data around a central value and checked for systematic dependence on the chosen central value. We typically use about 30 lattices per bare parameter value to do this. The resulting uncertainties are completely dominated by systematics, to be described below, so it is not worthwhile to work with larger datasets.

I. Z_A

Figure 2 illustrates our results for Z_A . It shows large scale views of Z_A for a 16^3 and a 24^3 spatial volume lattice. The 16^3 volume shows clear discretization artifacts above $a\mu \sim 1.4$. This represents an upper limit on the range of $a\mu$ values which can be analyzed. The finer grained 24^3 data do not have this issue.

Fits about some central value of $a\mu$ typically show a value close to unity with a statistical uncertainty of a few parts per mille. That Z_A is close to unity for the fermion action used here (nHYP) fermions has been well documented in the literature (cf. Ref. [46]).

However, there is another issue. Z_A should be a constant across $a\mu$ because the operator has no anomalous dimension. Our datasets show a small but noticeable drift of $Z_A(a\mu)$ versus $a\mu$. This is probably due to coupling to the pseudoscalar state, as described in the original literature [45]. We account for this drift by comparing linear fits to $Z_A(a\mu)$ versus $a\mu$ over windows of $a\mu$. We pick (somewhat arbitrarily) a central value $a\mu = 1$ and a range $a\mu = 0.8-1.2$. (For comparison, $\mu = 2$ GeV corresponds

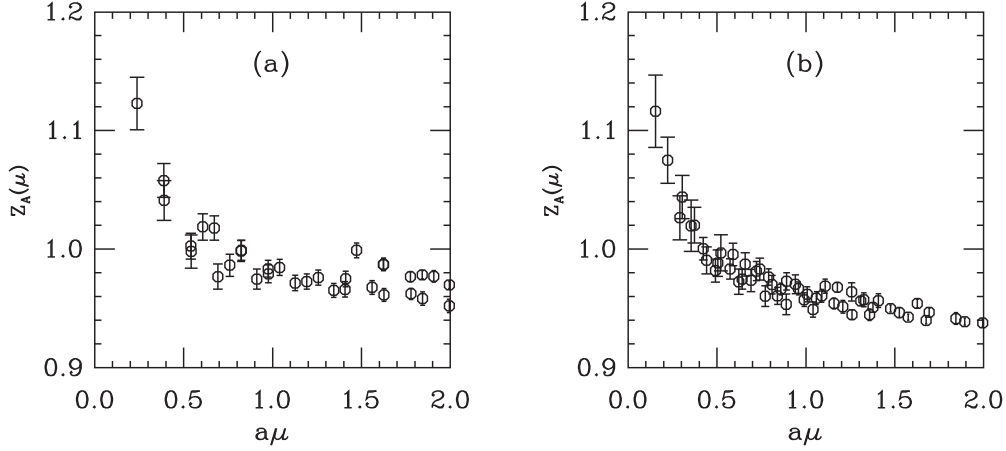


FIG. 2. Examples of datasets and results for Z_A . Panel (a) is from the $\beta = 5.35$, $\kappa = 0.12775$, $L = 16$ set and (b) from $\beta = 5.35$, $\kappa = 0.1282$, $L = 24$. They show Z_A versus $a\mu$ around $a\mu = 1$.

to $a\mu \sim 1.4$ at our coarsest lattice spacings down to 0.8 at our finest spacings.) Our systematic uncertainty is taken to be $|Z_A(a\mu = 1.2) - Z_A(a\mu = 0.8)|/2$. This gives a systematic uncertainty in the range of 0.005-0.008 as compared to statistical uncertainties from $Z_A(a\mu = 1)$ of 0.002-0.003. We use the first quantity as the uncertainty for Z_A .

2. Z_S and Z_m

Z_m is a bit more complicated to compute. We take Z_m from the renormalization factor for the scalar current Z_S^{RI} as $Z_m = 1/Z_S$, defined at some value of μa . We must then convert it to an $\overline{\text{MS}}$ value at a nominal scale $\mu = 2$ GeV. (This is done to make contact with pre-existing $SU(3)$ results.) This involves two steps after $Z_S^{RI}(a\mu)$ is determined; the analysis to determine this quantity is identical to what is done for Z_A . First, there is the conversion to $\overline{\text{MS}}$ at the scale at which Z_S^{RI} is determined. An explicit three loop formula (for general N_c and N_f fundamental representation fermions) for this conversion is given by Chetyrkin and Retey [47]. (See also Ref. [48].) To use it we need the $\overline{\text{MS}}$ coupling at scale $\mu = (\mu a)/a$. The lattice spacing is given by the flow parameter in lattice units ($t_0^L = t_0/a^2$ where $t_0 = 0.15$ fm from the compilation in Ref. [42]). The $\overline{\text{MS}}$ coupling comes from the plaquette, where in the ‘‘alpha-V’’ scheme [49,50]

$$\ln \frac{1}{N_c} \text{Tr} U_p = -4\pi C_F \alpha_V(q_V^*), \quad (43)$$

where $q^* = 3.41/a$ for the Wilson plaquette gauge action and $C_F = (N_c^2 - 1)/(2N_c)$ is the usual invariant. Then the conversion to $\overline{\text{MS}}$ is given by

$$\alpha_{\overline{\text{MS}}}(e^{-5/6} q^*) = \alpha_V(q^*) \left(1 - \frac{2}{3} N_c \frac{\alpha_V}{\pi} \right) \quad (44)$$

and run to $\alpha_{\overline{\text{MS}}}(2 \text{ GeV})$ with the usual two-loop formula

$$\alpha_s(q) = \frac{\alpha_s(q_0)}{v} \left(1 + \beta_1 \frac{\alpha_s(q_0)}{v} \log v \right) \quad (45)$$

with

$$v = 1 - \beta_0 \frac{\alpha_s(q_0)}{2\pi} \log \frac{q_0}{q}. \quad (46)$$

In all these equations β_0 and β_1 are the two lowest coefficients of the beta function. Recalling that $\beta_0 = 11/3N_c - 2/3N_f$ and $\beta_1 = 34/3N_c^2 - N_f/2((20/3)N_c + 4C_F)$, we note the appearance of the ‘t Hooft coupling $N_c \alpha_s$ in all these formulas. (The RI to $\overline{\text{MS}}$ formula, which we do not quote, involves $\alpha_s C_F$ as well.) We did not find Eq. (44) for $N_c \neq 3$ in the literature but it can be reconstructed from expressions in Ref. [51].

Finally, the $\overline{\text{MS}}$ Z_m is run to the final scale $\mu = 2$ GeV; this is done with the usual two loop formula

$$m_q(q) = m_q(\mu) \left(\frac{\alpha_s(q)}{\alpha_s(\mu)} \right)^{\frac{\gamma_0}{2\beta_0}} \left[1 + \frac{\alpha_a(q) - \alpha_s(\mu)}{4\pi} \times \left(\frac{\gamma_1 \beta_0 - \beta_1 \gamma_0}{2\beta_0^2} \right) \right]. \quad (47)$$

This is always a small effect since $\mu a \sim 1$ puts μ in close vicinity to 2 GeV already. The γ_i ’s are the one and two loop terms for the mass anomalous dimension.

The need to match and run makes the determination of Z_m much more fraught than the case of Z_A . The issue can be seen in the RI to $\overline{\text{MS}}$ conversion factor. (Here we describe the situation for $N_c = 3$.) Working at $a\mu \sim 1$, the scale μ ranges from about 1.4 to 2 GeV and $\alpha(\mu)$ is in the range 0.18–0.2. The conversion factor can be written as

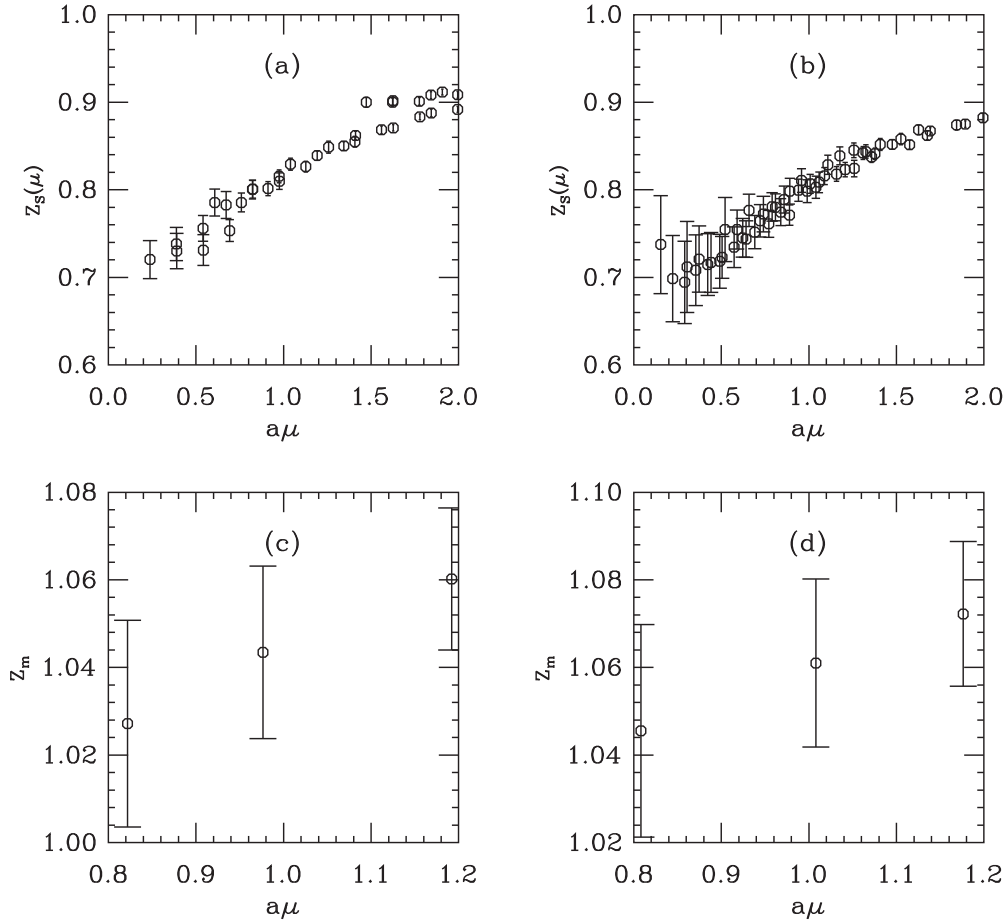


FIG. 3. Examples of datasets and results for Z_S and Z_m . Panels (a) and (c) are from $\beta = 5.35$, $\kappa = 0.12775$, $L = 16$ set and (b) and (d) from $\beta = 5.35$, $\kappa = 0.1282$, $L = 24$. Panels (a) and (b) show Z_S from lattice data versus $a\mu$ around $\mu = 1$ while panels (c) and (d) show $Z_m^{\overline{\text{MS}}}$ from linear fits to $Z_S(a\mu)$ centered at the shown $a\mu$ values, then converted into $Z_m^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$. The error bar includes the factor $C_3\alpha_s^3/R$, as a systematic.

$$R = 1 + \sum_i C_i \alpha_s^i. \quad (48)$$

The fraction of R from the highest order term, $C_3\alpha_s^3/R$, is about two percent (slightly bigger at smaller lattice spacing, slightly smaller at bigger lattice spacing, of course). This issue has already been noticed and described by Chetyrkin and Retey [47]. The suggested cure, to match at bigger $a\mu$, is not possible for our datasets due to the discretization effects we have already described. We must include a systematic effect in the error budget. We elect to do this by taking $C_3\alpha_s^3/R$ as a fractional systematic uncertainty on $m_q^{\overline{\text{MS}}}$. (Compare the discussion in Ref. [17], from a study at much smaller lattice spacing.) We again bracket the match between $a\mu = 0.8$ and 1.2.

We conclude with some figures showing the analysis for Z_m , in Fig. 3. The errors on $Z_m(\mu)$ are from the $C_3\alpha_s^3$ term.

One positive remark about $Z_m^{\overline{\text{MS}}}$ worth mentioning: the points shown at different $a\mu$ involve slightly different amounts of correction (since the conversion from Rl' to

$\overline{\text{MS}}$ is done at different $a\mu$ values with different running distances to $\mu = 2 \text{ GeV}$). Nevertheless, the results are reasonably independent of $a\mu$ even discounting the overall systematic uncertainty.

IV. FITTING STRATEGIES

We believe that little in our fitting strategy is novel. Fits involve minimizing a chi-squared function

$$\chi^2 = \sum_{ij} X^T(i) \frac{C(i,j)^{-1}}{\Delta E(j)\Delta E(j)} X(j), \quad (49)$$

where the sum runs over all quantities determined by simulation and the entries are $X(i) = E(i) - T(i)$ where $E(i)$ is the measured data value, $\Delta E(i)$ is its standard deviation of the mean, $T(i)$ is the model (containing parameters to be fit) and $C(i,j)$ is the correlation between the different experimental values. If the data points are

assumed to be uncorrelated, $C(i, j)^{-1} = \delta(i, j)$ in our convention.

We include correlations in Eq. (49) by jackknife. Recall that under a jackknife the average a quantity \bar{x} and its uncertainty Δx are given in terms of N individual jackknife averages $x(n)$

$$\begin{aligned}\bar{x} &= \frac{1}{N} \sum_n x(n) \\ (\Delta x)^2 &= \frac{N-1}{N} \frac{1}{N} \sum_n (x(n)^2 - \bar{x}^2).\end{aligned}\quad (50)$$

The correlation function is computed similarly, with a convention that the diagonal entries are the identity:

$$C(i, j) = \frac{1}{\Delta x_i \Delta x_j} \frac{N-1}{N} \sum_n (x_i(n) - \bar{x}_i)(x_j(n) - \bar{x}_j). \quad (51)$$

Recall all the ingredients we need: am_q , am_{PS} , af_L , t_0/a^2 , Z_A , Z_m . We combine these into dimensionless continuum-regulated quantities, which are then used as input data to fits which determine the LO and NLO chiral parameters. The dimensionless quantities we need, compulsively retaining the lattice spacing, are

$$\begin{aligned}\hat{m}_q &= Z_m \sqrt{\frac{t_0}{a^2}} am_q \\ \hat{m}_{\text{PS}}^2 &= \frac{t_0}{a^2} (am_{\text{PS}})^2 \\ \hat{f}_{\text{PS}} &= Z_a \sqrt{\frac{t_0}{a^2}} af_{\text{PS}}.\end{aligned}\quad (52)$$

In practice, only am_q , am_{PS} , and af_L show measurable correlations and we retain only these correlations in the chiral fits. The uncertainties on \hat{m}_q , \hat{f}_{PS} , and \hat{m}_{PS}^2 come from the uncertainties in their ingredients, combined in quadrature. We also need t_0/a^2 (actually, its inverse) as a (squared) lattice spacing to add lattice dependent terms in the chiral fits.

In Sec. III B we mentioned the issue that we have to perform a fit determining a set of parameters $\{a\}$ from $y(i) = f(x_i, \{a\})$, where both the y_i 's and x_i 's have uncertainties. We deal with that issue by promoting the x_i 's in the fitting function to additional terms in the χ^2 function. For example, in Sec. III B the y_i 's were values of $t_0 \pm \Delta t_0$ at a set of N bare parameter values, and the x_i 's were a set $\xi_i \pm \Delta \xi_i$. The set $\{a\}$ were a set of J coefficients on a polynomial fit. We expand the χ^2 function to

$$\chi^2 = \sum_{i=1}^N \frac{(y_i - f(X_i, \{a\}))^2}{(\Delta y(i))^2} + \sum_{i=1}^N \frac{(x_i - X_i)^2}{(\Delta x(i))^2} \quad (53)$$

(we suppress the obvious correlation term), so that we now have $2N$ terms in χ^2 and $J + N$ quantities to be determined. If there were no errors on the x_i the counting of degrees of

freedom would be $N - J$, and with the procedure we have outlined it is still $2N - (J + N) = N - J$.

The ξ fits present one final annoyance, since the fitting function must be written entirely in terms of quantities to be fit. This means that in Eq. (18) we must remove the error-bearing m_{PS}^2 from the right-hand side of these expressions. We do this by adding a $(y(i) - T(i)) = (m_{\text{PS}}(i)^2 - M_{\text{PS}}(i)^2)$ term to the chi-squared formula. For N_d bare parameter values there will be $3N_d$ data points (F_{PS} , m_q and M_{PS}) to be fit, with $4 + 3N_d$ fit parameters, for $N_d - 4$ degrees of freedom.

Finally, we must discuss how we deal with lattice artifacts. Our lattice action has order a^2 artifacts, and this means that the LEC's which will come out of fits will also carry $O(a^2)$ corrections. In principle, for x fits, that will be the case for all four LO and NLO parameters and the three additional NNLO ones. To include all these correction terms in the fitting function would be very unwieldy (and, given our uncertainties, quite unstable). Instead, we follow the lead of Ref. [17] and proceed empirically, adding terms and seeing how they affect the χ^2 of a fit. We discover that we are sensitive to lattice artifacts in two places, basically a modification of the right-hand sides of Eqs. (10), (17), and (18). To be explicit, we fit the following functional forms. For x fits,

$$\begin{aligned}m_{\text{PS}}^2 &= \left(1 + c_B \frac{a^2}{t_0}\right) 2Bm_q \left[1 - \frac{1}{2}x \left(\log \frac{\mu_\pi^2}{M^2} + l_3\right) \right. \\ &\quad \left. + x^2 \left(\frac{17}{8}T_M^2 + k_M\right)\right] \\ f_{\text{PS}} &= \left(1 + c_F \frac{a^2}{t_0}\right) F \left[1 + x \left(\log \frac{\mu_\pi^2}{M^2} + l_4\right) \right. \\ &\quad \left. + x^2 \left(-\frac{5}{4}T_F^2 + k_F\right)\right],\end{aligned}\quad (54)$$

T_F and T_M are given by Eq. (11). The NLO ξ fitting functions become

$$\begin{aligned}f_{\text{PS}} &= \left(1 + c_F \frac{a^2}{t_0}\right) \frac{F}{2} \left[1 + \left(1 + 4 \frac{m_{\text{PS}}^2}{8\pi^2 F^2}\right) \right. \\ &\quad \left. \times \left(\ln \frac{\mu^2}{m_{\text{PS}}^2} + l_4\right)\right]^{1/2} \\ m_q &= \left(1 + c_B \frac{a^2}{t_0}\right) \frac{m_{\text{PS}}^2}{2B} \left[1 + \frac{1}{2} \left(\frac{m_{\text{PS}}^2}{8\pi^2 \mathcal{F}(F, l_4, m_{\text{PS}}^2)}\right) \right. \\ &\quad \left. \times \left(\log \left(\frac{\mu^2}{m_{\text{PS}}^2}\right) + l_3\right)\right].\end{aligned}\quad (55)$$

Note again that all input variables (m_q , M_{PS}^2 , F_{PS}) have been rescaled by the appropriate power of t_0 . This means that an NLO fit involves six parameters and NNLO, nine. Of these two nuisance parameters, c_B is much more important. (It was the only term kept by Ref. [17].) We comment on their values in the next section.

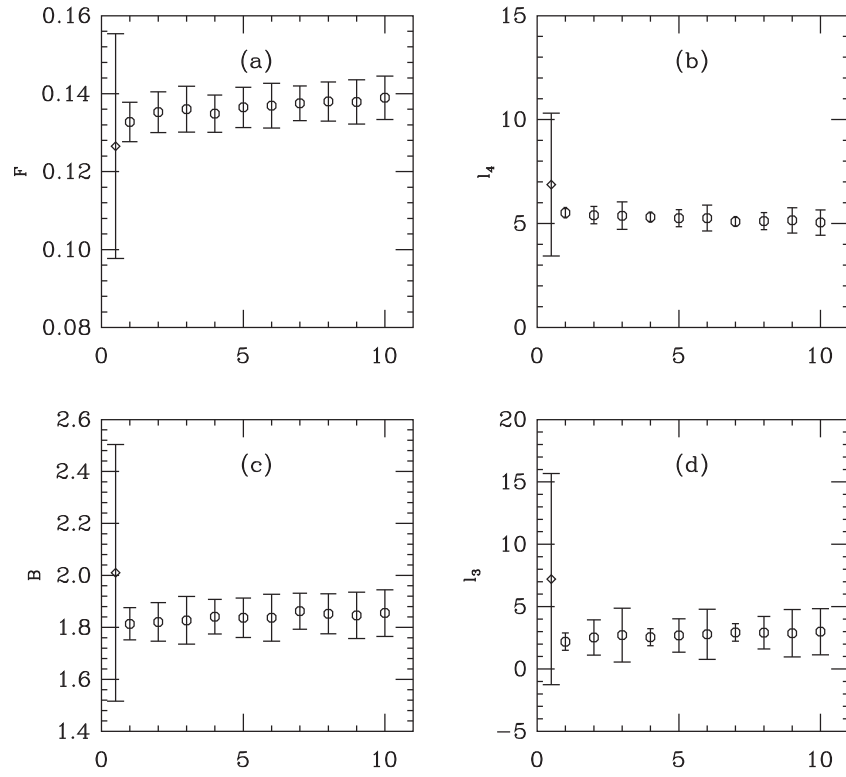


FIG. 4. Fit values of LO and NLO chiral parameters from an NNLO x fit to $N_c = 5$ over a set of priors for l_{12} , k_F , and k_M . The diamond shows the fit result without priors.

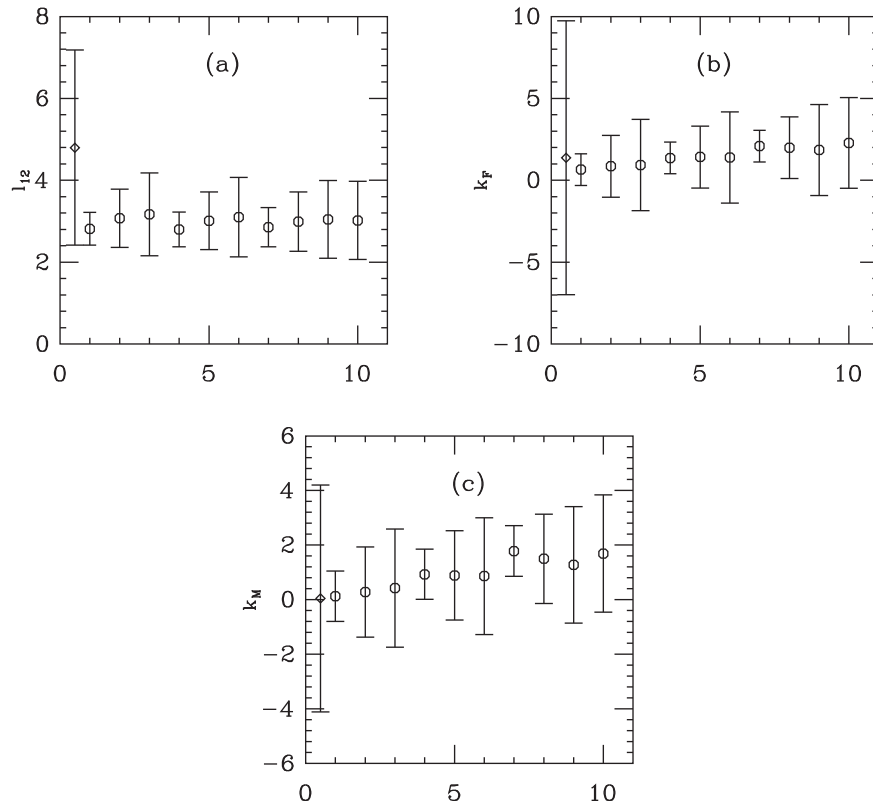


FIG. 5. Fit values of NNLO parameters l_{12} , k_F , and k_M from NNLO x fits to $N_c = 5$ over a set of priors for them. The diamond shows the fit result without priors.

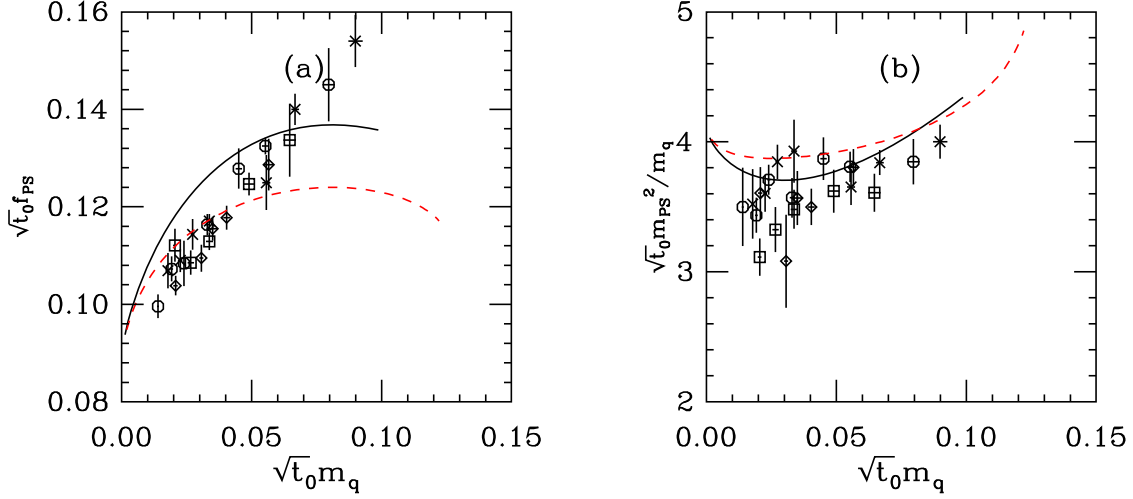


FIG. 6. $N_c = 3$ data compared to NLO formulas from the x -parameterization in the black solid lines black and the ξ parameterization in red dashes with “known” (FLAG) [16] parameters for the LEC’s. (a) $\sqrt{t_0} f_{\text{PS}}$ versus $\sqrt{t_0} m_q$; (b) $\sqrt{t_0} m_{\text{PS}}^2 / m_q$ versus $\sqrt{t_0} m_q$. Symbols show $\beta = 5.25$ in squares, $\beta = 5.3$ in diamonds, $\beta = 5.35$ in octagons, $\beta = 5.4$ in crosses.

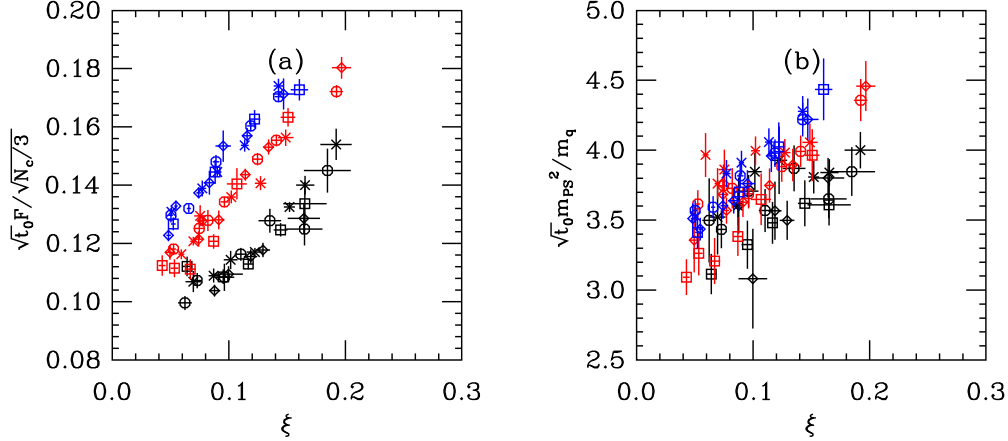


FIG. 7. Plots of (a) $\sqrt{t_0} f_{\text{PS}} / \sqrt{N_c/3}$ and (b) $\sqrt{t_0} m_{\text{PS}}^2 / m_q$ versus $\xi = m_{\text{PS}}^2 / (8\pi^2 f_{\text{PS}}^2)$. Colors label different N_c values (black for $N_c = 3$, red for $N_c = 4$ and blue for $N_c = 5$), and the different symbols label the different bare gauge couplings as described in the text.

Priors are included in the standard way, as additional terms in the χ^2 function, $\chi^2 \rightarrow \chi^2 + \chi_P^2$ where

$$\chi_P^2 = \sum_j \frac{(P_j - \bar{P}_j)^2}{\Delta P(j)^2}. \quad (56)$$

We discover that while both x and ξ NLO fits are uniformly stable over a wide range of choices of fit parameters, the NNLO fits are unstable without inclusion of priors. We made a set of fits with a broad range of priors for l_{12} , k_F , and k_M , and we found that values of the four fitted LO and NLO quantities are reasonably independent of the choices we made, but the fitted values and (especially) their uncertainties of l_{12} , k_F , and k_M are completely determined by the priors. This result occurs for all N_c ’s. We present one illustration, for $N_c = 5$. This is a fit to the datasets with the

smallest 15 values of ξ . Figure 4 shows the LO and NLO quantities for ten choices of priors, set identical for l_{12} , k_F , and k_M . The values, from left to right, are $(P, \Delta P) = (0.0, 1.0), (0.0, 2.0), (0.0, 3.0), (1.0, 1.0), (1.0, 2.0), (1.0, 3.0), (2.0, 1.0), (2.0, 2.0), (2.0, 3.0), (3.0, 3.0)$. The fitted values for l_{12} , k_F , and k_M are shown in Fig. 5. In our NLO fits in Sec. V, we will keep the (1.0,2.0) prior.

We remark in passing that one lattice artifact which we looked for but did not observe was an extra term in the relation $m_{\text{PS}}^2 = 2Bm_q$ due to nonzero lattice spacing. This is an extra term on the right hand side of the first equation in the set of Eq. (54). We checked this most thoroughly for NNLO x fits. The addition of terms $m_{\text{PS}}^2 = 2Bm_q(\dots) + C_a(a^2/t_0)$ or $m_{\text{PS}}^2 = 2Bm_q(\dots) + C_a(a/\sqrt{t_0})$ make a tiny change to the χ^2 (comparing the same fit ranges) compared to leaving them out.

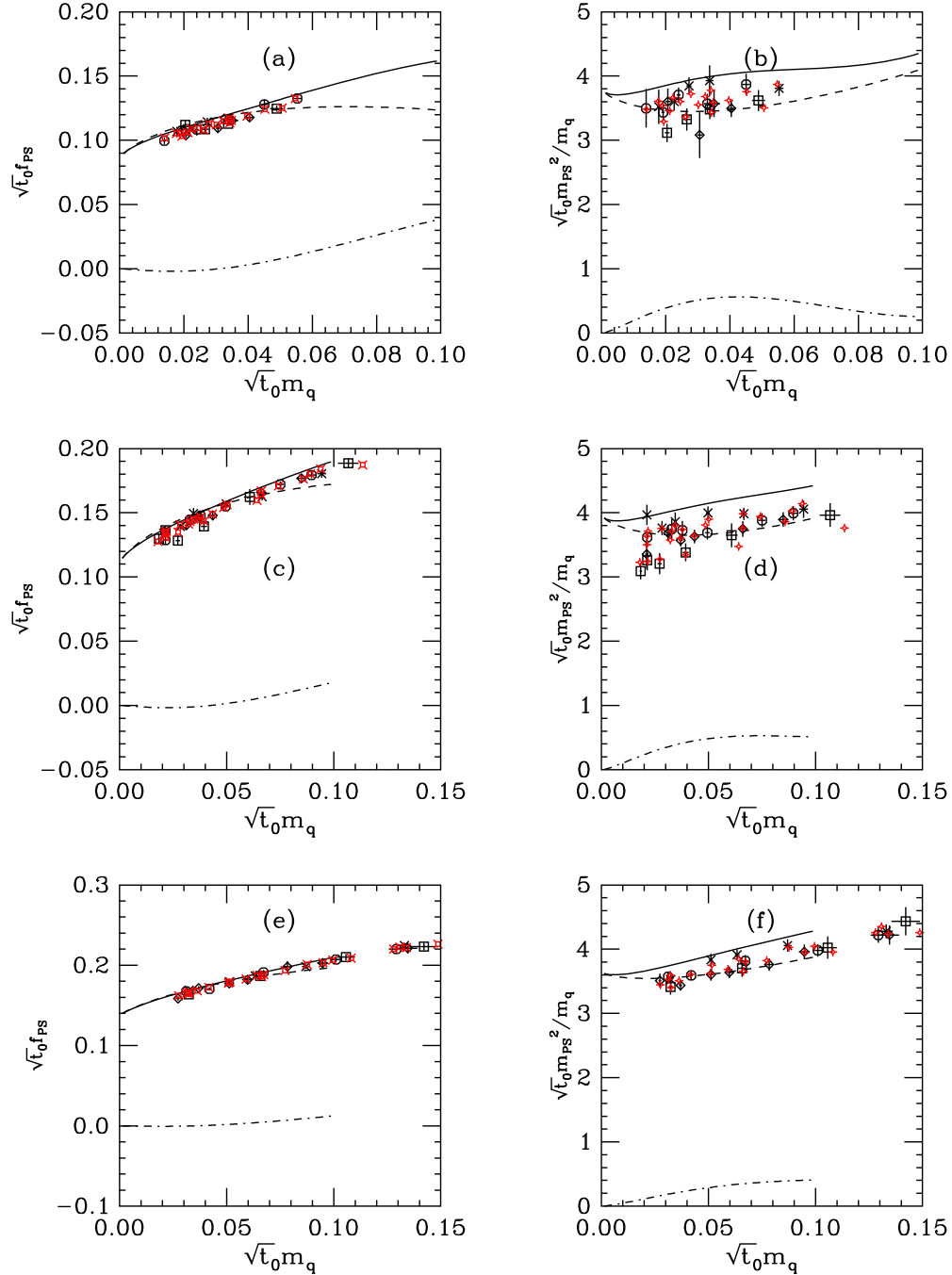


FIG. 8. NNLO x fits showing $\sqrt{t_0} f_{\text{PS}}$ and $\sqrt{t_0} m_{\text{PS}}^2 / m_q$ vs $\sqrt{t_0} m_q$. (a) and (b) show $N_c = 3$, (c) and (d) show $N_c = 4$, and (e) and (f) show $N_c = 5$ datasets. The fits involve the seven parameters of the NNLO expression, with the NNLO LEC's stabilized by priors as described in the text and two $O(a^2)$ correction terms as described in Eq. (54). The different plotting symbols label the different beta values of the datasets and are given in the text. Red points are the fitted values associated with the black data points. The lines show the continuum limit of the fitting functions. The decomposition of the $SU(N_f)$ fitting functions for f_{PS} and m_{PS}^2 / m_q (shown as solid lines) is split into their NLO (dashed lines) and NNLO (dash-dotted lines) components.

All that happens is that the uncertainties on the other fit parameters (mostly F) grow and the central values drift by a σ or so. A broad prior on C_a is needed to stabilize the fit. The authors of Ref. [17] use an action with smeared gauge links which is similar to ours and do not include this term either.

V. RESULTS FROM FITS TO CHIRAL PERTURBATION THEORY

A. $SU(2)$ chiral perturbation theory

Our extraction of LEC's from our datasets is done by performing a series of fits varying the range of quark

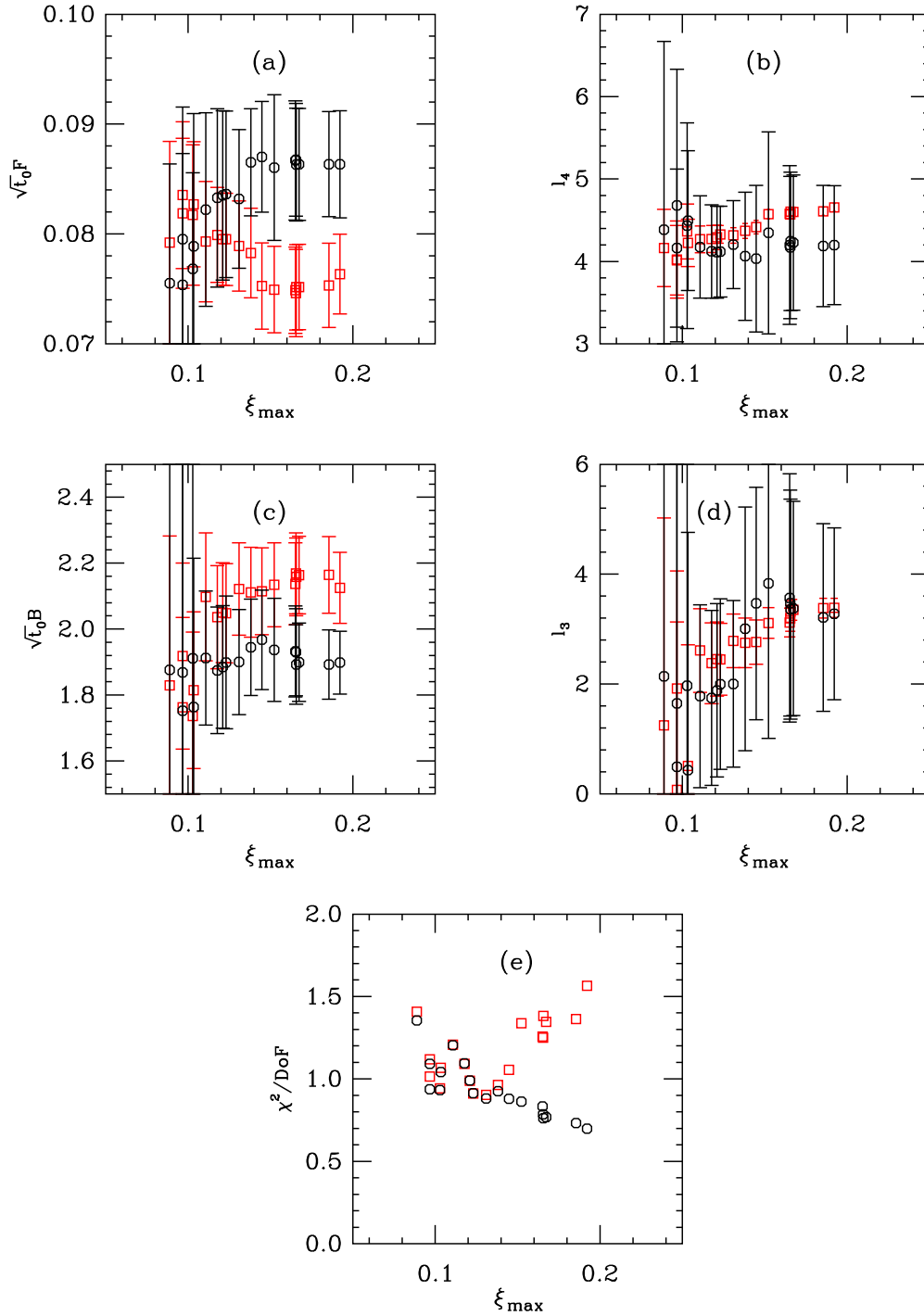
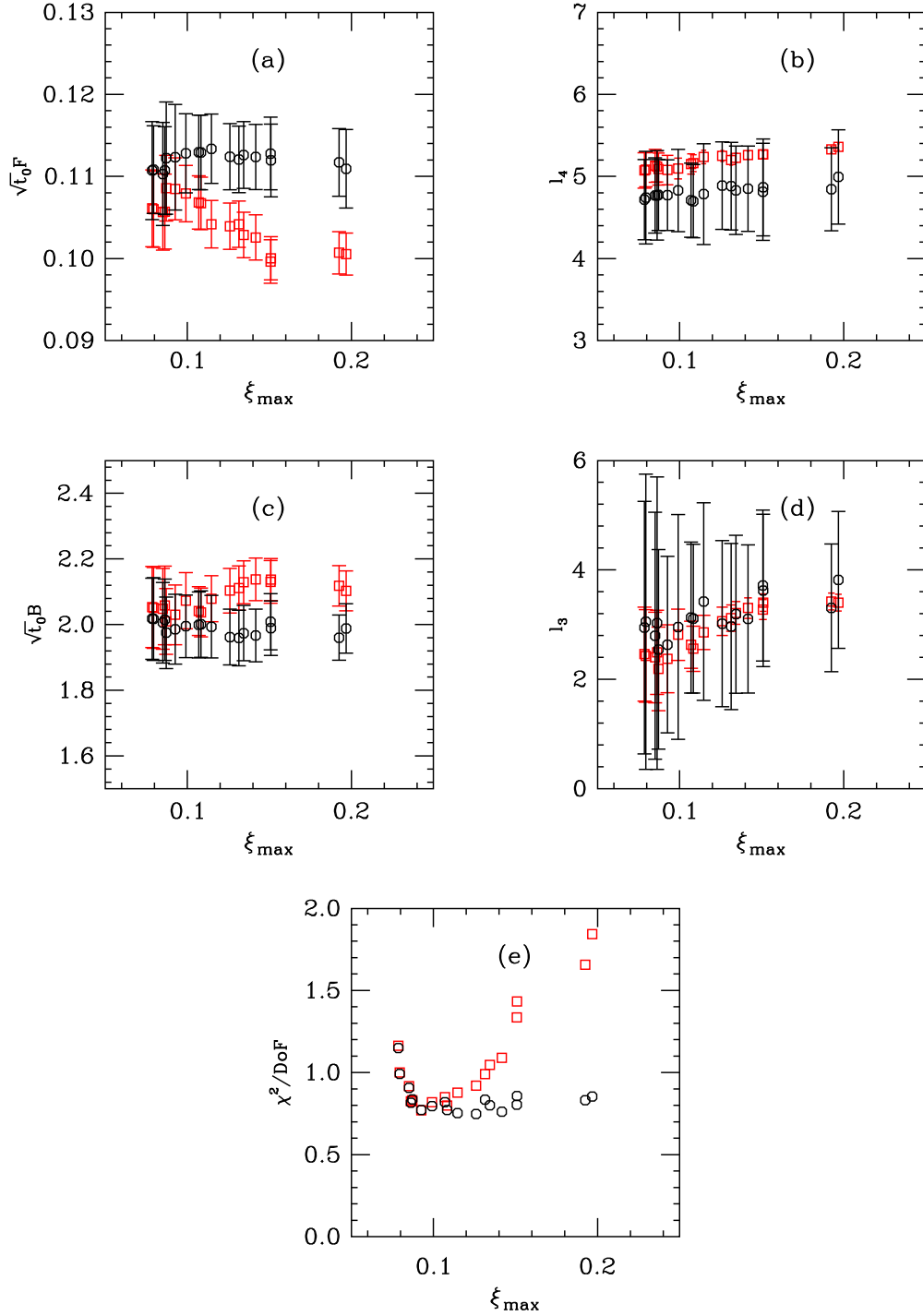


FIG. 9. Results of NLO and NNLO $SU(2)$ x fits to $N_c = 3$ datasets versus ξ_{\max} . The red squares show NLO fits and the black octagons show NNLO fit results. (a) $\sqrt{t_0}F$, (b) l_4 , (c) $\sqrt{t_0}B$, (d) l_3 , (e) the χ^2 per degree of freedom.

masses, typically varying the maximum value of ξ in the dataset and using model averaging to produce a set of results. The lattice data for f_{PS} and m_{PS}^2 are typically very smooth functions of the quark mass. The fitting functions are also very smooth. It is usually possible to get a good quality fit for any ξ range. The issue is then whether the fit parameters are stable under variation of fit ranges.

The values of $SU(N_f)$ LEC's were already a closed subject before we began our project. They are summarized by FLAG [16] and come from datasets of much higher quality than ours. The study of $N_c > 3$ is our goal. We therefore use $N_c = 3$ as a fiducial: can we reproduce FLAG results?

Recall that we are scaling all quantities with the appropriate power of t_0 to produce dimensionless


 FIG. 10. Results of NNLO x fits to $SU(4)$ datasets versus ξ_{\max} , as in Fig. 9.

quantities. The 2019 FLAG review tells us that $F = 87$ MeV (in the “93 MeV” convention) so with $\sqrt{t_0} = 0.15$ fm, $\hat{F} = \sqrt{2} \times 87 \text{ MeV} \times 0.15 \text{ fm} \sim 0.09$ in our convention. The condensate $\Sigma = F^2 B$ in the same convention. The review quotes $\Sigma^{1/3} \sim 266(10)$ MeV (in $\overline{\text{MS}}$ at $\mu = 2$ GeV) and with $\hat{F} = 0.09$, $\hat{B} \sim 2.05$. The review lists $l_3 = 3.41(82)$ and $l_4 = 4.40(28)$.

Before doing any fits, we can just compare our data to NLO curves with these values for the LEC’s. Figure 6 shows two plots: $\sqrt{t_0} f_{\text{PS}}$ versus $\sqrt{t_0} m_q$ in panel (a) and $\sqrt{t_0} m_{\text{PS}}^2 / m_q$ versus $\sqrt{t_0} m_q$ in panel (b). The different plotting symbols correspond to different values of the bare gauge coupling.

The figure shows one loop results with the FLAG parameters for the LEC’s. The black curves show the

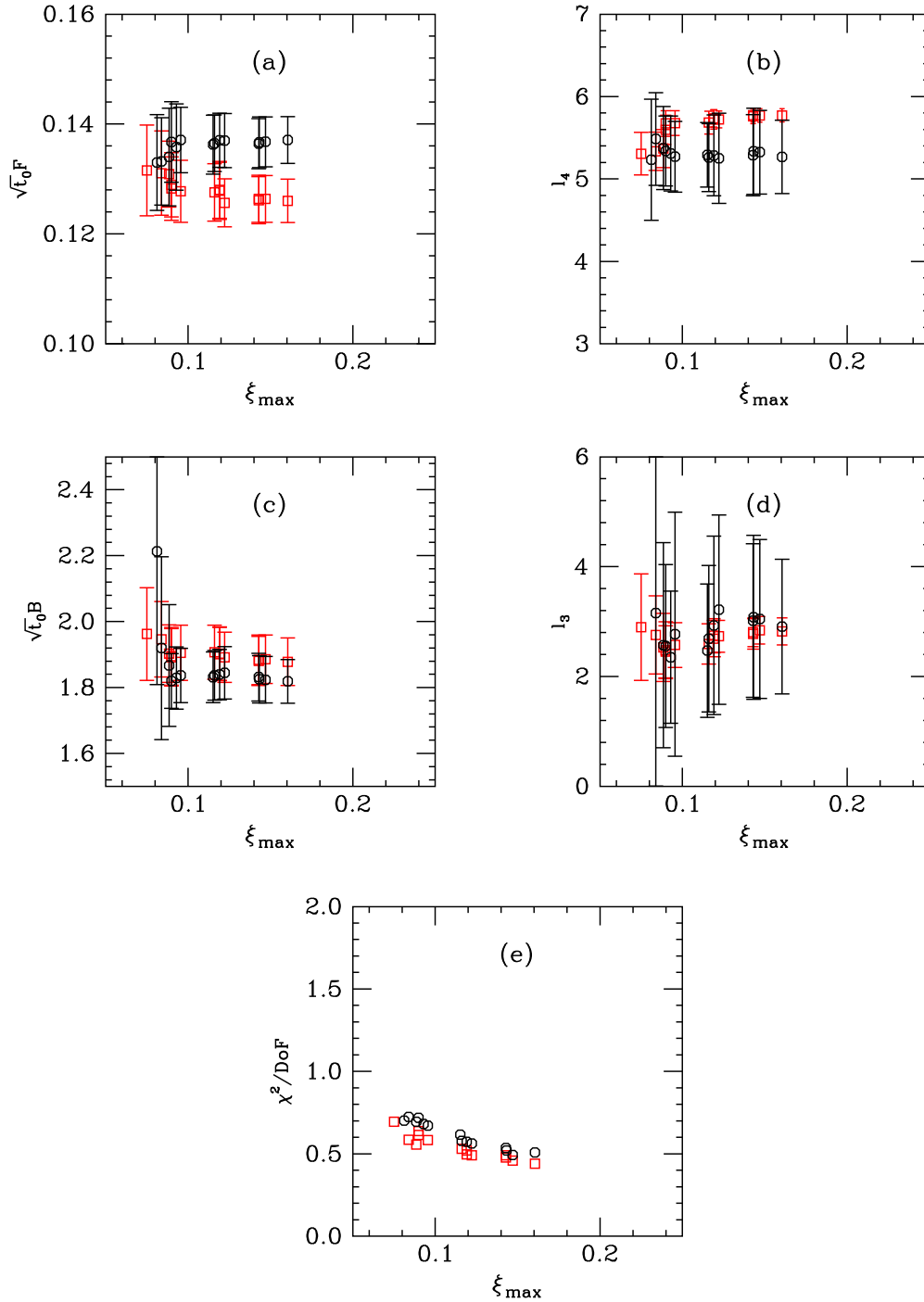


FIG. 11. Results of NNLO x fits to $SU(5)$ datasets versus ξ_{\max} , as in Fig. 9.

NLO x curve while the dashed red curves the NLO ξ curve. The data, especially for f_{PS} , are much straighter than either NLO fit would favor. In an NLO fit to the data, the fit parameter for l_4 will drift upward as higher mass points are kept, to try to straighten the curve. The datasets we collected mostly lie outside the range where NLO chiral perturbation theory is applicable. To fit all our datasets it is necessary to do NNLO fits.

As a second preliminary picture we display $\sqrt{t_0}f_{\text{PS}}/\sqrt{N_c/3}$ and $\sqrt{t_0}m_{\text{PS}}^2/m_q$ versus ξ , in Fig. 7. The quantities

plotted on the x and y axes of these plots are quite degenerate, but the figure does display the landscape of the data. The different plotting symbols label the different beta values (and hence different lattice spacings) of the datasets. The catalog is

- (i) For $N_c = 3$, shown in black, squares for $\beta = 5.25$, diamonds show $\beta = 5.3$, octagons show $\beta = 5.35$, crosses show $\beta = 5.4$.
- (ii) For $N_c = 4$, shown in red, squares are for $\beta = 10.0$, diamonds for $\beta = 10.1$, octagons for $\beta = 10.2$, crosses for $\beta = 10.3$.

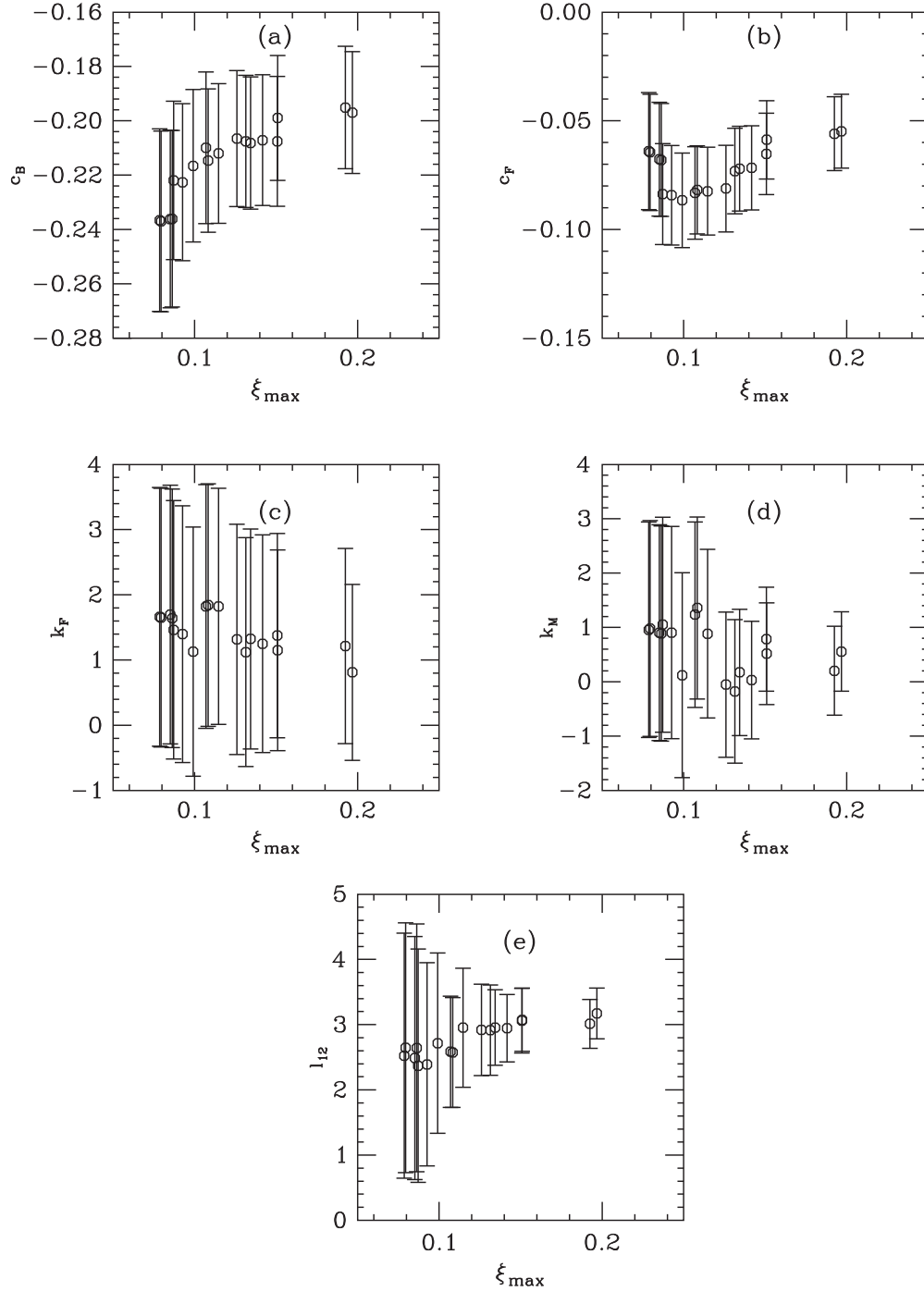


FIG. 12. More results of NNLO x fits to $SU(4)$ datasets versus ξ_{\max} : (a) c_B , the a^2 correction to B (b) c_F , the a^2 correction to F , and the three NNLO LEC's (controlled by priors in the fits) (c) k_F , (d) k_M , (e) l_{12} .

- (iii) For $N_c = 5$, shown in blue, squares are for $\beta = 16.2$, diamonds for $\beta = 16.3$, octagons for $\beta = 16.4$, crosses for $\beta = 16.6$.

We begin with a set of typical results for NNLO x fits, Fig. 8. The data in these fits has been selected to be less than some chosen value of ξ_{\max} . The fits involve the seven parameters of the NNLO expression, with the

NNLO LEC's stabilized by priors as described in the text, and two $O(a^2)$ correction terms as given in Eq. (54). The two sets of points show $\sqrt{t_0}m_{\text{PS}}^2/m_q$ and $\sqrt{t_0}f_{\text{PS}}$ vs $\sqrt{t_0}m_q$. The different plotting symbols label the different beta values (and hence different lattice spacings) of the datasets as we have listed. The red points are the fit values associated with each data point.

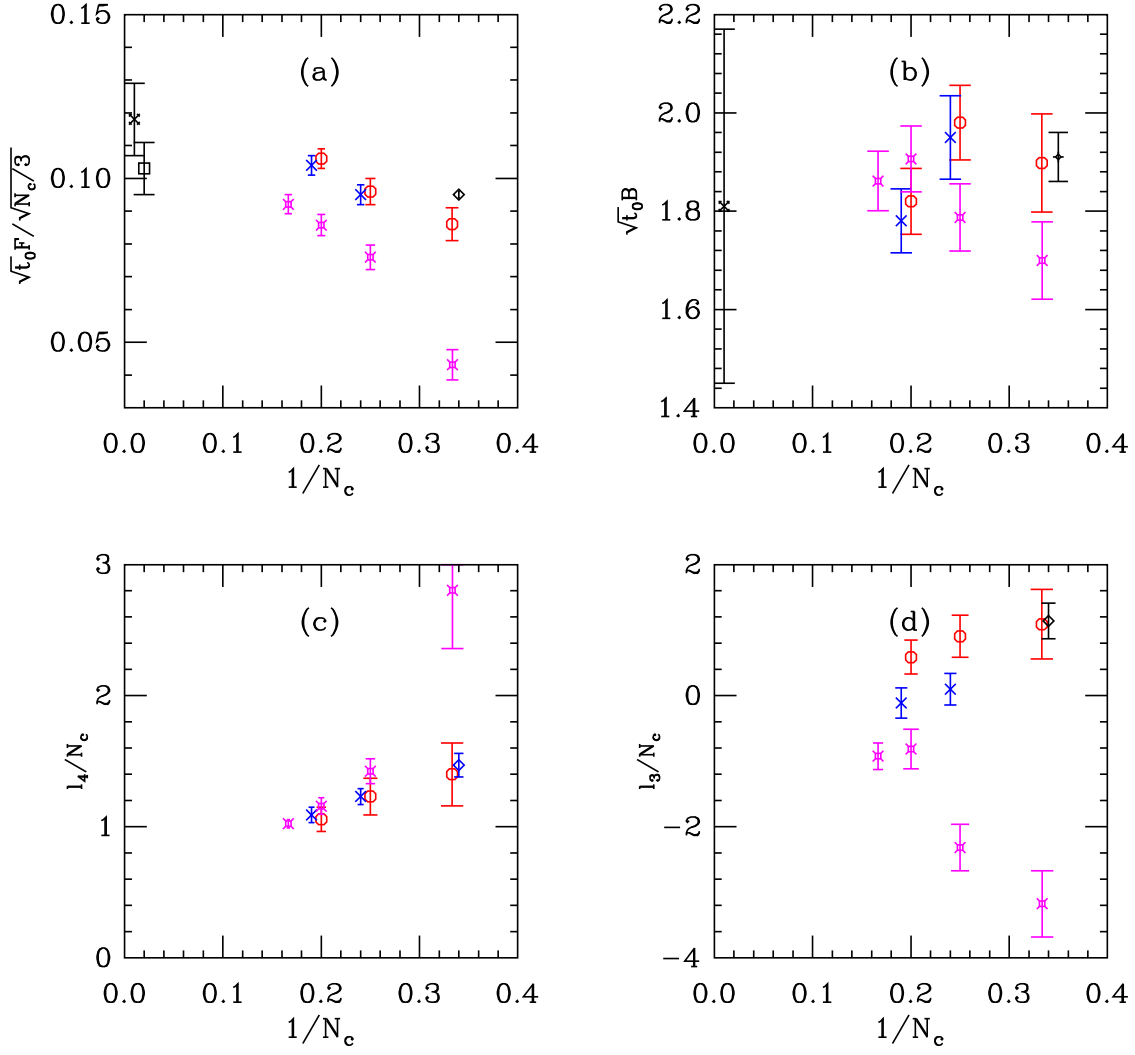


FIG. 13. LEC's from fits of NNLO $SU(2)$ chiral perturbation theory for $N_c = 3, 4,$ and 5 , along with other relevant results for comparison. (a) $\sqrt{t_0 F} / \sqrt{N_c/3}$, (b) $\sqrt{t_0 B}$, (c) l_4/N_c , (d) l_3/N_c . The plotting symbols are red octagons, for our $SU(2)$ results; blue crosses, our $U(2)$ results, converted to $SU(2)$ LEC's. Other relevant data are also shown (in black). High precision $N_f = 2$, $N_c = 3$ results are diamonds [16], and fancy diamonds, [17]. There are two large N_c limits of quenched data, the large volume results of [52] as squares and the small volume ones of [53,54] as fancy crosses. Purple fancy squares show $N_f = 4$ results from [18].

The solid lines are the continuum result. The difference between the line and the data points is due to the nuisance parameters c_F and c_B in Eq. (54).

To determine the LEC's, we organized a set of NNLO fits by sorting each N_c 's data into a file with increasing ξ and performed a series of fits beginning with a subset of points with the smallest ξ values and extending up to some maximum ξ . We monitored the χ^2 per degree of freedom and confidence level of the fits. Figure 9 shows results from $N_c = 3$ for B , F , l_3 , and l_4 , along with the chi-squared per degree of freedom. The flatness of the fit quantities versus ξ_{\max} indicates that we can perform model averaging over our suite of fits to determine the LEC's.

Figures 10 and 11 show the same information, but for $N_c = 4$ and 5 . We show one representative example of our determination of the cutoff dependent terms c_B and c_F and the NNLO parameters k_F , k_M , and l_{12} , for $N_c = 4$, in Fig. 12. Recall that the NNLO fitted parameters are strongly controlled by priors.

Results are listed in Table V and displayed in Fig. 13.

The uncertainties on l_3 are much larger than those of l_4 . This is similar to what is seen in the FLAG averages for $N_c = 3$ [16].

As a final check of the consistency of our results, we break apart the NNLO predictions for f_{PS} and m_{PS}^2/m_q into their LO + NLO and NNLO components and plot them.

TABLE V. LO and NLO LEC's of $SU(2)$ chiral perturbation theory from our $N_c = 3, 4$, and 5 datasets.

	$N_c = 3$	$N_c = 4$	$N_c = 5$
$\sqrt{t_0}B$	1.90(10)	1.98(8)	1.82(7)
$\sqrt{t_0}F$	0.086(5)	0.111(5)	0.137(4)
l_4	4.2(7)	4.9(6)	5.2(4)
l_3	3.2 ± 1.5	3.62 ± 1.3	2.9 ± 1.3
c_B	-0.14(3)	-0.20(2)	-0.14(4)
c_F	-0.6(2)	-0.06(2)	-0.04(3)
l_{12}	2.7(5)	3.1(4)	3.3(5)
k_F	1.14 ± 1.5	1.0 ± 1.4	1.5 ± 1.8
k_M	0.15 ± 1.0	0.4 ± 0.8	0.5 ± 1.0

This is shown in Fig. 8. The NNLO piece remains small over the range of $\sqrt{t_0}m_q$ values used in fits.

B. $U(2)$ chiral perturbation theory

The analysis path for $U(2)$ chiral fits exactly parallels that for $SU(2)$. We performed fits to the NLO and NNLO formulas, studying individual N_c datasets. We included additional nuisance parameters to account for finite lattice spacing effects. Specifically,

$$m_{\text{PS}}^2 = \left(1 + c_B \frac{a^2}{t_0}\right) (M_{\text{NLO}}^2 + M_{\text{NNLO}}^2)$$

$$f_{\text{PS}} = \left(1 + c_F \frac{a^2}{t_0}\right) (F_{\text{NLO}} + F_{\text{NNLO}}) \quad (57)$$

where the NLO and NNLO terms are given in Eqs. (24) and (25). The NLO fits involve six parameters $B, F, l_3^{(0)}, l_4^{(0)}, c_B$ and c_F . The NNLO fits add two more: T_F and T_M , for eight parameters, and replaces the $l_i^{(0)}$'s by $l_i^{(0)} + l_i^{(1)}/N_c$.

We need one more input parameter, the quenched topological susceptibility χ_T . Reference [55] measured it to be

$$t_0^2 \chi_T = 7 \times 10^{-4}. \quad (58)$$

(See also [56] for earlier determinations of χ_T .)

We experimented with priors for T_F and T_M . We discovered that if the fitting range in ξ or $\sqrt{t_0}m_q$ was large, no priors were needed, while when the range became small, setting a prior 0.2 ± 0.2 for T_F and -0.2 ± 0.2 for T_M stabilized the fit.

Notice that the NLO fits are ‘‘fits to a straight line’’ (plus lattice artifacts) of our data.

As in the case of the $SU(2)$, we can generally find fits which have low chi-squares to any dataset; the issue is whether the fit parameters are stable under dataset size. A second consideration is whether the fit makes sense in that the NNLO contribution is small compared to the NLO one.

$N_c = 3$ is a special case: $U(2)$ chiral fits fail. This can be seen in Fig. 14, where we break up a typical NNLO fit into its component parts. For $N_c = 3$ the actual NNLO component is huge compared to the NLO piece. The fitted B also has a very large uncertainty as it tries to compensate for the incorrect functional form demanded by the fitting function. We include the data with the same plotting symbols as in Fig. 8.

This leaves us $N_c = 4$ and 5. Figure 14 shows that the size of the various contributions is consistent with a small NNLO correction and that the situation is more improved for $N_c = 5$ than for $N_c = 4$.

We proceed to results. Figures 15 and 16 show results of individual NLO and NNLO fits out to values of ξ_{max} . The NLO fits drift when ξ_{max} becomes greater than about 0.1. These fits will be model-averaged once a range is chosen. We then compare NLO and NNLO fits at $\xi_{\text{max}} = 0.107$ with NNLO fits at $\xi_{\text{max}} = 0.20$ ($N_c = 4$) or NLO and NNLO fits at $\xi_{\text{max}} = 0.09$ with NNLO fits at $\xi_{\text{max}} = 0.16$ ($N_c = 5$). Fitted values for the LEC's agree at the one standard deviation level. Results from the NNLO fits at large ξ_{max} are listed in Table VI.

One final thing we must do is connect the $U(2)$ LEC's to the $SU(2)$ ones. The F values need no conversion. The other LEC's need a shift and rescaling according to Eqs. (27) and (9). With the dimensionless $U(2)$ scheme point $\mu = t_0(8\pi^2 F^2) = 0.64$ and the $SU(2)$ $\mu = t_0 m_\pi^2(\text{phys}) = 0.011$, the converted expressions are recorded in Table VI. As we saw in the $SU(2)$ case, the results for l_3 are quite a bit noisier than the ones for l_4 .

C. Discussion of results

We collect our results in a panel of figures, Fig. 13. Our results are presented in $\overline{\text{MS}}$ at a scale of 2 GeV (equivalent, for $N_c > 3$, of course) and we have converted the l_i 's to a scale $\mu^2 = m_\pi^2$. The $U(2)$ parameters have been matched to $SU(2)$ ones, so the plots show $SU(2)$ LEC's.

We have included data from other sources. At $N_c = 3$ these are the FLAG [16] numbers. They do not quote a direct average for B so we substitute the measurement of B from Ref. [17] as comparison.

We also added two $N_c \rightarrow \infty$ results, from the large N_c —small volume simulations of Refs. [53,54] and from the large volume quenched simulations of Ref. [52].

Quenched simulations, of course, fall outside the two chiral expansions ($SU(N_f)$ and $U(N_f)$) we have studied: the quenched pseudoscalar decay constant has no chiral logarithm and the dependence of the pseudoscalar mass on the fermion mass is not $m_{\text{PS}}^2 \propto m_q$ but

$$m_{\text{PS}}^2 \propto m_q^{1/(1+\delta)}. \quad (59)$$

These differences are related to the fact that in the quenched approximation, the flavor singlet pseudoscalar meson propagator is not a pole; it is a double pole involving

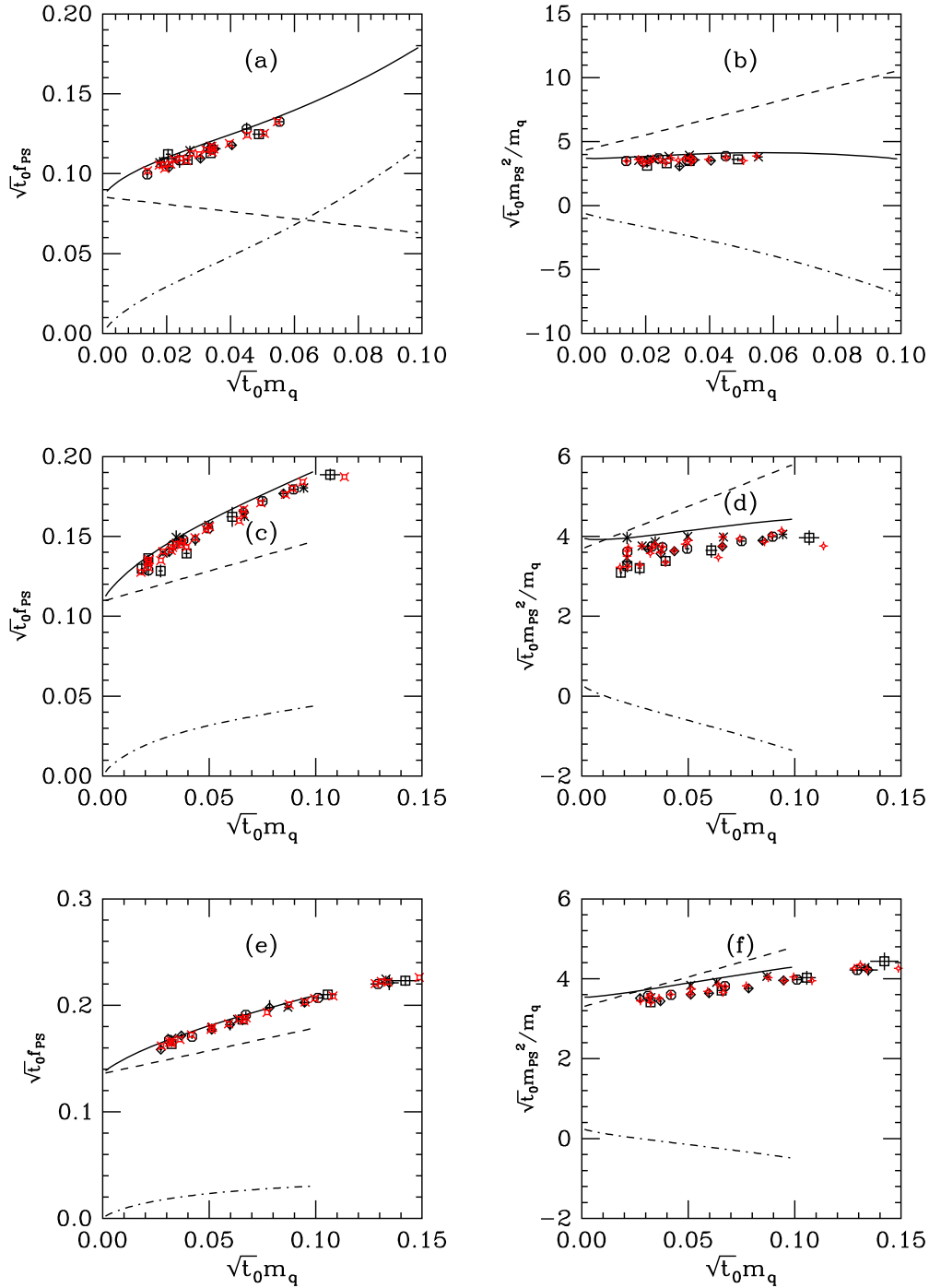


FIG. 14. Decomposition of the $U(N_f)$ fitting functions for f_{PS} and m_{PS}^2/m_q (shown as solid lines) into their NLO (dashed lines) and NNLO (dash-dotted lines) components. (a) and (b) $N_c = 3$; (c) and (d) $N_c = 4$; (e) and (f) $N_c = 5$. The data are shown with the same plotting symbols as in Fig. 8.

two ordinary pseudoscalars—a “hairpin” [44]. There is no sense in which the flavor singlet pseudoscalar’s mass decreases with N_c , as occurs with any $N_f \neq 0$. We are not sure how to add quenched results to the panels showing l_3 and l_4 of Fig. 13. Still, the coupling of the hairpin, like the coupling to the tadpole which gives the chiral logarithm, scales as $1/F^2 \sim 1/N_c$ and disappears in the limit.

It seems reasonable to expect that quenched QCD and QCD with any fixed number of flavors of dynamical fermions should share a common large N_c limit. However, the N_c dependence of observables away from the limit will depend on N_f . What one learns from doing simulations which include dynamical fermions, of course, involves the fermions. It is expected that their effects fall

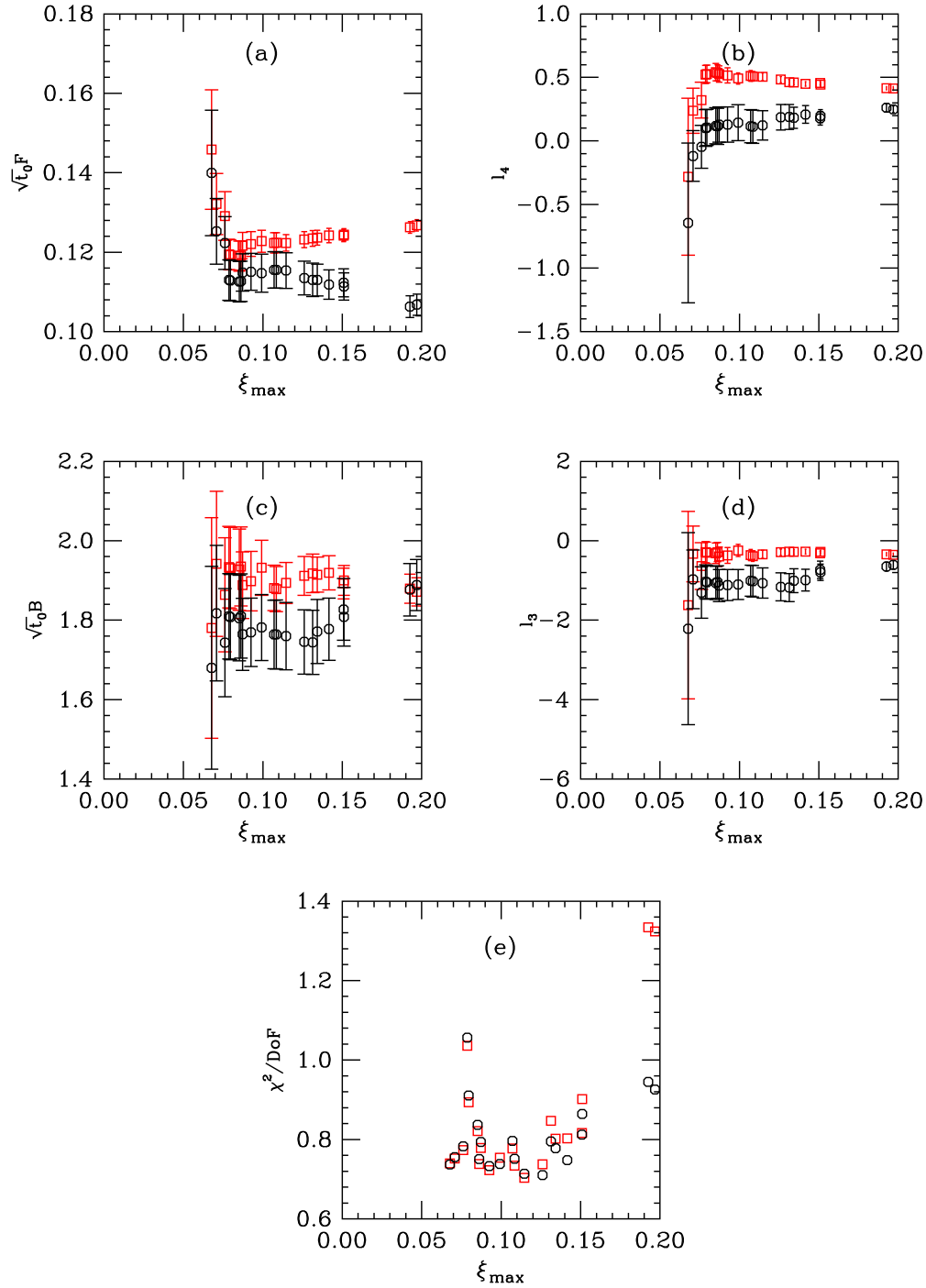


FIG. 15. Results of NLO (red squares) and NNLO (black octagons) $U(2)$ fits to $N_c = 4$ datasets versus ξ_{\max} . (a) $\sqrt{t_0}F$, (b) $l_4^{(0)}$ or $l_4^{(0)} + l_4^{(1)}/N_c$, (c) $\sqrt{t_0}B$, (d) $l_3^{(0)}$ or $l_3^{(0)} + l_3^{(1)}/N_c$, (e) l_3 , (e) the χ^2 per degree of freedom.

away, but (for example) do some contributions disappear (say, as a power of $1/N_c$) independently of N_f , or in terms of the ratio N_f/N_c , or does something else happen? We think this question is as interesting as asking what are the large N_c limits of B and $F/\sqrt{N_c}$.

The authors of Refs. [53,54] performed simulations in the context of the twisted Eguchi-Kawai matrix

model at $N_c = 169, 289, \text{ and } 361$ at several lattice spacings per N_c . They give the large N_c limiting results $\sqrt{8t_0\sigma} = 1.078(9)$ and $f_{\text{PS}}/\sqrt{\sigma}\sqrt{3/N_c} = 0.22(1)(2)$ where σ is the string tension and the two uncertainties are statistical and systematic. They use the “93 MeV” definition for the decay constant, so we convert their numbers to

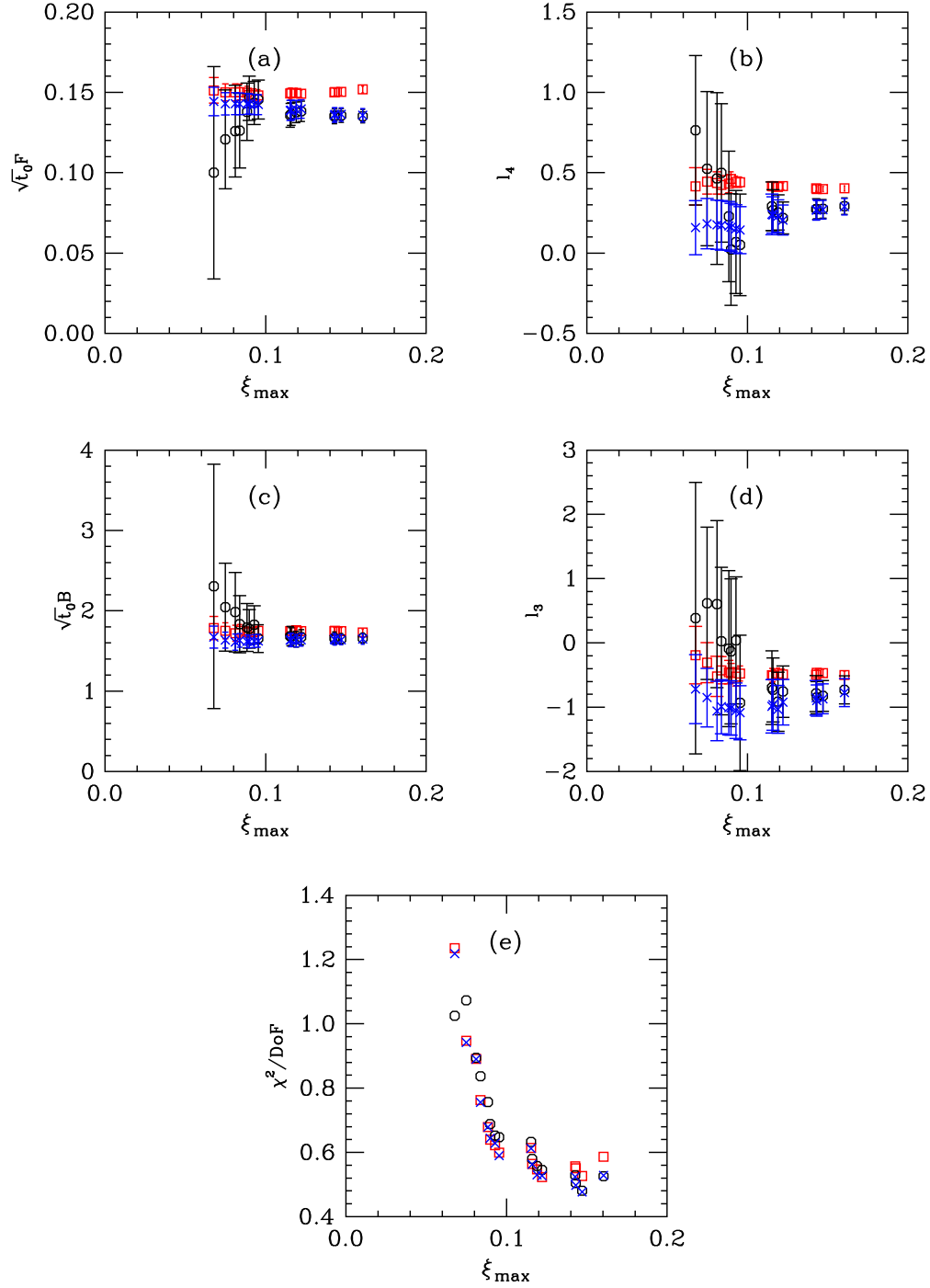


FIG. 16. Results of NLO and NNLO $U(2)$ fits to $N_c = 5$ datasets versus ξ_{\max} . The red squares are NLO fits, the black octagons are NNLO fits without priors, and the blue crosses are NNLO fits with priors. (a) $\sqrt{t_0}F$, (b) $l_4^{(0)}$ or $l_4^{(0)} + l_4^{(1)}/N_c$, (c) $\sqrt{t_0}B$, (d) $l_3^{(0)} + l_3^{(1)}/N_c$, (e) the χ^2 per degree of freedom.

$$\sqrt{\frac{3}{N_c}}\sqrt{t_0}F = \sqrt{2}\left[\frac{F}{\sqrt{\sigma}}\frac{\sqrt{8t_0\sigma}}{\sqrt{8}}\right] = 0.118(11) \quad (60)$$

(combining errors in quadrature for the plot). Reference [54] quotes $\sqrt{t_0}B = 1.81(36)$ as a byproduct of their value of Σ (which has a much smaller uncertainty).

Reference [52] has quenched data for $N_c = 2-7$ and 17, at one lattice spacing, $a \sim 0.1$ fm. They quote a large N_c limit of

$$\frac{1}{\sqrt{2}}\sqrt{\frac{3}{N_c}}\frac{F}{\sqrt{\sigma}} = 0.2174(30) \quad (61)$$

TABLE VI. LO and NLO LEC's of $U(2)$ chiral perturbation theory from our $N_c = 4$ and 5 datasets. The “converted” columns show conversions to $SU(2)$ quantities according to Eq. (27). In the column we have listed l_3 and l_4 ; note the rescaling.

	$N_c = 4$	converted	$N_c = 5$	converted
$\sqrt{t_0}B$	1.84(9)	1.96(10)	1.65(6)	1.79(7)
$\sqrt{t_0}F$	0.109(4)		0.136(4)	
$l_4^0 + l_4^{(1)}/N_c$	0.22(6)	4.93(24)	0.28(6)	5.45(30)
$l_3^{(0)} + l_3^1/N_c$	-0.74(24)	-0.57 ± 1.15	-0.81(23)	-0.11 ± 0.23
c_B	-0.20(2)		-0.14(4)	
c_F	-0.06(2)		-0.04(3)	
T_F	0.08(5)		0.06(4)	
T_M	-0.06(7)		-0.07(6)	

with an additional eight per cent error on the string tension, which is the dominant uncertainty. With a choice of $\sqrt{\sigma} = 440$ MeV and $t_0 = 0.15$ fm, this is the limiting value

$$\lim_{N_c \rightarrow \infty} \sqrt{\frac{3}{N_c}} \sqrt{t_0} F = 0.103(8). \quad (62)$$

We note that the authors of Ref. [52] extrapolate all their data in $1/N_c^2$.

Next, we attempt a comparison with the results of Hernandez *et al.* [18]. Their $N_f = 4$ datasets are fit to $U(4)$ chiral perturbation theory and they perform interpolations in N_f assuming that N_f appears in the combination N_f/N_c (so that tuning N_c is a proxy for varying N_f).

They have tables of $aF/\sqrt{N_c}$ which we convert to $\sqrt{t_0}\sqrt{3/N_c}F$ in our conventions using $\sqrt{t_0} = 0.15$ fm and their $a = 0.075$ fm. Their $N_f = 4$ results are lower than our $N_f = 2$ ones. The coefficient of N_f/N_c in their fitting function is negative and their $N_f = 2$ extrapolations are 0.093(3) for $N_c = 3$, 0.101(3) for $N_c = 4$ and 0.105(3) for $N_c = 5$. Their extrapolation to infinite N_c is 0.124(3)—0.130(3) for the two functional forms they use.

We present $\sqrt{t_0}B = Z_s\sqrt{t_0}/a(aB)$ from their tables, converted to the $SU(N_f)$ B , in Fig. 13(b). There seems to be little N_f dependence on this quantity—which their N_f/N_c parametrizations also show.

We translated their data for L_F into $l_4(\mu = m_\pi^2)$ by

$$l_4(N_f = 4, \mu) = \log \frac{8\pi^2 F^2}{m_\pi^2} + \frac{64\pi^2}{(N_f/2 = 2)} L_F. \quad (63)$$

Figure 13(c) shows that their $N_f = 4$ results for $N_c > 3$ are consistent with ours. Their prediction of $N_c = 3$, $N_f = 2$ numbers ($l_4 = 5.1(3)$ or $4.1(11)$ for two fits) are consistent with ours.

Finally, l_3 . We again convert their $U(4)$ quantity to an $SU(4)$ one and plot it in panel d of Fig. 13. This quantity is

apparently strongly N_f dependent, in addition to being very noisy. They quote an $N_c = 3$, $N_f = 2$ value of $l_4 = 0.4 \pm 1.6$ (at $\mu = m_\pi$) to be compared with our 3.2 ± 1.5 and FLAG's 3.41(82).

It's a bit dangerous to extrapolate our data to $N_c \rightarrow \infty$, we think. But (just to save readers the work of doing it themselves) a linear fit to the $SU(2)$ values for $\sqrt{t_0}B$ and $\sqrt{t_0}\sqrt{3/N_c}F$ of the form $c_1 + c_2/N_c$ gives large N_c values of $\sqrt{t_0}B = 1.72(22)$ and $\sqrt{t_0}\sqrt{3/N_c}F = 0.136(10)$. A glance at Fig. 13 shows that these predictions seem to be unexpected. Of course, a convincing plot would benefit from continuum predictions from all the possible approaches (listed at the beginning of the paper) to the large N_c limit. Presumably all approaches would converge to the same large N_c limit, but would do so in different ways, which might illustrate how varying numbers of fermion flavors affect the LEC's.

VI. CONCLUSIONS

The results shown in Fig. 13 show that we have not answered the list of questions which motivated this project, though we may have made a start:

- (1) How do the low energy constants of the chiral effective theory scale with N_c ? What is their limit?

The expected leading scaling $B \sim N_c^0$, $F \sim \sqrt{N_c}$, $l_3, l_4 \sim N_c$ seem to hold. We can see subleading N_c behavior in F , l_3 , and l_4 . With three values of N_c we cannot say anything about corrections beyond $1/N_c$.
- (2) Is there a crossover to $U(2)$ chiral behavior?

This we cannot tell. $U(2)$ fits fail for $N_c = 3$. We see that in our $N_c = 4$ and 5 datasets both chiral expansions give comparable results for the LEC's, when they are converted to a common scheme. We are aware of no direct calculations of the mass of the flavor singlet meson for $N_c > 3$, so the $U(2)$ fitting functions depend on the validity of the Witten–Veneziano relation.

What could we have done better (and why)? The list is obvious: smaller fermion masses would have been a big help, to be able to do chiral fits deeper in the NLO regime. This then implies a need for bigger lattice volumes, so as not to be compromised by finite size effects. Fortunately, the larger the value of N_c , the less this is an issue. Our large lattice spacings led to big uncertainties in the value of lattice to continuum matching factors, and the $SU(3)$ literature makes the obvious point that smaller lattice spacing allows more controlled matching at larger momentum scales. And finally, more values of N_c would certainly have been helpful. Trying to extrapolate three values of N_c leaves little room to deal with the possibility that quantities scale nonlinearly in $1/N_c$. We suspect, though, that datasets of the size of the ones reported in FLAG for $SU(3)$ could complete the story of the chiral and continuum limit of large N_c QCD.

Of course, to really give high precision answers to the questions we have asked will probably involve some kind of superanalysis involving a variety of approaches including simulations at several fixed N_f values, as well as quenched simulations in small and large volumes. But in

the meantime, we think that the low-statistics take away continues to be that $N_c = 3$ QCD is not that different from its large N_c limit.

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