Pion and Kaon Physics with Improved Staggered Quarks

THE MILC COLLABORATION

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Motivation

Masses and decay constants of light pseudoscalars can be measured on the lattice (at fixed $m_{\rm quark}$ and a) with high precision: statistical errors are $\sim$0.1–0.4% in our calculation.

Assuming chiral and continuum extrapolations can be performed accurately, such a calculation:

- Provides sensitive check of algorithms and methods by comparing f_π and f_K to experiment; tests $\sqrt[4]{\rm Det}$ trick and understanding of "taste" violations.
- Allows us to extract coefficients of the $\mathcal{O}(p^4)$ chiral Lagrangian (the Gasser-Leutwyler L_i).
- Makes possible a determination of the light quark masses (requires perturbative or non-perturbative evaluation of mass renormalization constant).

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Simulations

- Three light dynamical flavors, with various values of $m_u = m_d \equiv m_q$, and strange quark mass held fixed at nominal value, m_s.
- Asqtad action: one-loop + tadpole Symanzik improved gauge [1]; tree-level + tadpole improved staggered quarks [2].
- Errors: $\mathcal{O}(\alpha_S a^2)$ in general. Taste-violations require 2-gluon exchange, are $\mathcal{O}(\alpha_S^2 a^2)$.
- Two lattice sets: lattice spacing ≈ 0.12 fm ("coarse") and ≈ 0.09 fm ("fine"). Table 1 shows the lattice parameters used.
- In this poster, m_s always means the s quark mass value used in simulations ($am_s = 0.05$ or 0.031). Values turn out to be higher than physical value, $m_s^{\rm phys}$:

$$\begin{aligned} m_s &\approx 1.18\, m_s^{\rm phys} \qquad [\text{coarse}] \\ m_s &\approx 1.10\, m_s^{\rm phys} \qquad [\text{fine}] \end{aligned} \tag{1}$$

- Relative scale among coarse (or, separately fine) lattices kept fixed using length r_1 [3, 4] from static quark potential. Reduce statistical fluctuations in r_1/a by using "smoothed" r_1/a coming from fit to smooth function:

$$\log(r_1/a) = C_0 + C_1(10/g^2 - 7) + C_2\, am_{\rm tot} + C_3\,(10/g^2 - 7)^2\,, \tag{2}$$

where $m_{\rm tot} = 2m_q + m_s$. Fit is good over our range of g^2 and m_{tot}.

- Absolute scale from Υ $2S$-$1S$ or $1P$-$1S$ splittings, determined by HPQCD group [5], on coarse 0.01 / 0.05 and fine 0.0062 / 0.031 lattices. We extrapolate to continuum linearly in $\alpha_S a^2$ and get $r_1 = 0.317(7)$ fm. (Scale is $\approx 9\%$ bigger than from using $r_0 = 0.5$ fm.)

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Table 1: Lattice Parameters

a (fm)	am_q / am_s	$10/g^2$	size	volume	number
0.12	0.03 / 0.05	6.81	$20^3\times 64$	$(2.5\ {\rm fm})^3$	262
0.12	0.02 / 0.05	6.79	$20^3\times 64$	$(2.5\ {\rm fm})^3$	485
0.12	0.01 / 0.05	6.76	$20^3\times 64$	$(2.5\ {\rm fm})^3$	608
0.12	0.007 / 0.05	6.76	$20^3\times 64$	$(2.5\ {\rm fm})^3$	447
0.12	0.005 / 0.05	6.76	$24^3\times 64$	$(3.0\ {\rm fm})^3$	137
0.09	0.00124 / 0.031	7.11	$28^3\times 96$	$(2.4\ {\rm fm})^3$	531
0.09	0.00062 / 0.031	7.09	$28^3\times 96$	$(2.4\ {\rm fm})^3$	583

The lattice sets above the double line are "coarse;" those below are "fine."

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Propagator Calculations: Sources

Have tried both point (P) and wall (W) operators at source and sink.

- "Wall" is quark source summed over the entire spatial slice, fixed to Coulomb gauge.
- At sink, "point" means usual local pseudoscalar density operator, summed over spatial slice,

$$\mathcal{O}_P(t) = \sum_{\vec x} \bar\psi^a(\vec x,t)(-1)^{\vec x + t}\psi^a(\vec x,t)\,, \tag{3}$$

where ψ is staggered field and a is color.

- At source, "point" is quark source with random $U(1)$ phase, summed over spatial slice $\Rightarrow$ non-local contributions cancel on average.
- Figure 1 is sample effective mass plot.
- Note that WP and PW amplitudes are equal, a consistency check.
- Finding masses from WW propagators is almost hopeless. Including excited state helps, but statistical errors get large.
- We therefore extract masses & decay constants from simultaneous fit (single exponentials) to WP and PP propagators. WP dominates determination of the mass; amplitude of PP gives decay constant.
- Minimum time distance for fit: 20 (coarse), 30 (fine).

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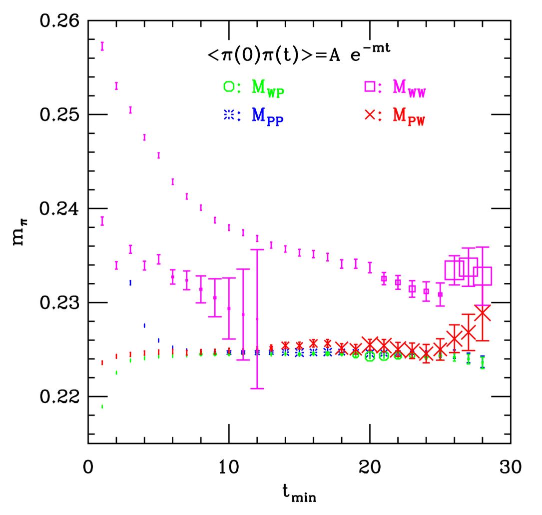
Figure 1



Pion masses with either point or wall at source or sink. For example, M_{PW} is effective mass with point source and wall sink. The lower set of "WW" points include an excited state in the fit. Symbol size is proportional to confidence level of the fit, with symbol size in the labels corresponding to 50%. Data is from coarse 0.01 / 0.05 lattice.

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Propagator Calculations: Details

- Compute propagators every 6 time units, with 2 sources per lattices.
- To reduce autocorrelations, block propagators from 4 successive lattices (24 time units) before fitting.
- On coarse lattices, find propagators for 9 valence masses between $0.1m_s$ and m_s. Construct pseudoscalars for all mass combinations, degenerate and non-degenerate.
- Repeat for fine lattices, but for 8 valence masses between $0.14m_s$ and m_s.
- Using jackknife, compute complete covariance matrix of data on each lattice set. Include correlations of decay constants with masses, as well as among masses and among decay constants.

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Taste Violations: Splittings

- Figure 2 shows splittings between pions of various tastes on the coarse lattices. These are all flavor-*charged*, *i.e.*, π^+ mesons. Therefore there are no contributions from disconnected graphs, even for the taste-singlet π_I^+
- "Accidental" $SO(4)$ identified by Lee and Sharpe [6] clearly operable: near degeneracy between π_{05}^+ and π_{i5}^+, between π_{0i}^+ and π_{ij}^+, and between π_0^+ and π_i^+.
- Fit in Fig. 2 is to tree level chiral form: linear in quark mass, but with constant splittings for all non-Goldstone particles. Splittings and slope determined from this fit $\Rightarrow$ input to NLO terms in chiral log fits (see below).
- On fine lattices, splittings have same form but ~ 0.4 times the size. Consistent with expectation of taste violations as $\mathcal{O}(\alpha_S^2 a^2)$: using $\alpha_S = \alpha_V(q^*)$ at one-loop [7] and $q^* = 3.33/a$,

$$(\alpha_S^2 a^2)_{\rm fine}/(\alpha_S^2 a^2)_{\rm coarse} \approx 0.375 \tag{4}$$

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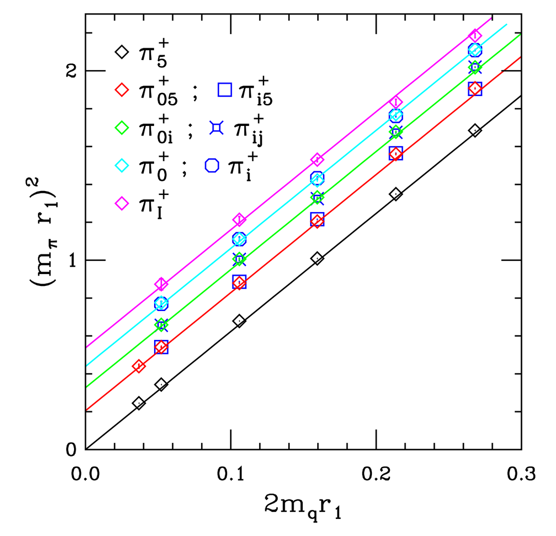
Figure 2



Charged π masses for various tastes on the coarse lattices. Tastes that are degenerate by $SO(4)$ symmetry are fit together.

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Taste Violations: Theory at NLO

- Lee and Sharpe [6] found chiral Lagrangian for a single staggered field at $\mathcal{O}(m, a^2)$, where m is a generic quark mass. Lagrangian includes the effects of taste violations.
- Aubin and Bernard [8, 9, 10] have generalized Ref. [6] to n staggered flavors and shown how to accommodate the $\sqrt[4]{\rm Det}$ trick in loop calculations. Result is staggered chiral perturbation theory, SχPT. (See talk by C. Aubin in *Hadron Spectrum and Quark Masses II* session.)
- One-loop chiral logs and analytic terms have been calculated in SχPT for Goldstone meson masses [8] and decay constants [9]. Partially quenched results are included, so all forms needed to fit current MILC data are available. From here on, let valence quark masses be m_x and m_y; sea quark masses are $m_u = m_d \equiv m_q$ and m_s.
- Express chiral logs in terms of function $\ell(M^2)$:

$$\ell(M^2) \equiv M^2\left(\ln\frac{M^2}{\Lambda_\chi^2} + \delta_1(ML)\right)\,, \tag{5}$$

where Λ_χ is the chiral scale, L is the spatial volume, and $\delta_1(ML)$ is the finite volume correction [10].

- Two examples of NLO [$\mathcal{O}(m^2, ma^2, a^4)$] chiral logs follow.

(1) K mass ($m_x = m_q$, $m_y = m_s$) [8]:

$$\frac{(m^{\rm 1-loop}_{K_5^+})^2}{m_x+m_y} = \mu\Bigg\{1 + \frac{1}{16\pi^2 f^2}\Bigg(\Bigg[-\frac{2a^2\delta'_V}{m^2_{\eta'_V} - m^2_{\eta_V}}\Big(\ell(m^2_{\eta_V}) - \ell(m^2_{\eta'_V})\Big)\Bigg] + \Big[V\to A\Big] + \frac{2}{3}\ell(m^2_{\eta_I})\Bigg) + \frac{16\mu}{f^2}(2L_8 - L_5)(m_x+m_y) + \frac{32\mu}{f^2}(2L_6 - L_4)(2m_q+m_s) + a^2 C\Bigg\}. \tag{6}$$

L_i are $\mathcal{O}(p^4) = \mathcal{O}(m^2)$ Gasser-Leutwyler parameters. δ'_V is a new chiral parameter; governs mixing of flavor-neutral, taste-vector, mesons through hairpins. Similar parameter, δ'_A, comes in flavor-neutral, taste-axial-vector channel. C is a new analytic parameter from taste-violating $\mathcal{O}(ma^2)$ operators. η_I is usual η in taste-singlet (I) channel; η_V, η'_V (η_A, η'_A) are corresponding mesons in taste-vector (-axial) channels. Normalization of f is such that $f_\pi \approx 131$ MeV.

(2) f_π ($m_x = m_y = m_q$) [9]:

$$f^{\rm 1-loop}_{\pi_5^+} = f\Bigg\{1 + \frac{1}{16\pi^2 f^2}\Bigg[2a^2\delta'_V\Bigg(\frac{m^2_{S_V} - m^2_{\eta_V}}{(m^2_{\pi^0_V} - m^2_{\eta_V})(m^2_{\eta'_V} - m^2_{\eta_V})}\ell(m^2_{\eta_V}) + \frac{m^2_{S_V} - m^2_{\eta'_V}}{(m^2_{\pi^0_V} - m^2_{\eta'_V})(m^2_{\eta_V} - m^2_{\eta'_V})}\ell(m^2_{\eta'_V}) + \frac{m^2_{S_V} - m^2_{\pi^0_V}}{(m^2_{\eta_V} - m^2_{\pi^0_V})(m^2_{\eta'_V} - m^2_{\pi^0_V})}\ell(m^2_{\pi^0_V})\Bigg) + \Big(V\to A\Big) - \frac{1}{16}\sum_B\Big(2\ell(m^2_{\pi^0_B}) + \ell(m^2_{K^+_B})\Big)\Bigg] + \frac{8\mu}{f^2}L_5(m_x+m_y) + \frac{16\mu}{f^2}L_4(2m_q+m_s) + a^2F\Bigg\}. \tag{7}$$

B runs over all 16 meson tastes; m_{S_V} is the mass of the ss meson with vector taste; F is another new analytic parameter from taste-violating $\mathcal{O}(ma^2)$ operators.

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NNLO Terms

Data very precise $\Rightarrow$ must go beyond NLO to get good fits. We include all NNLO analytic, physical parameters, *i.e.*, all analytic terms of $\mathcal{O}(m^3)$. NNLO chiral logs and taste-violating analytic terms are unknown and not included. But for larger masses, where NNLO terms are non-negligible, logs should be changing slowly $\Rightarrow$ well represented by analytic terms. Similarly, for larger masses, $\mathcal{O}(m^3)$ terms should be more important than taste-violating $\mathcal{O}(m^2a^2)$ or $\mathcal{O}(ma^4)$ terms.

Express NNLO terms in "natural" units, so that coefficients will be $\lesssim 1$ if chiral perturbation theory (χPT) well behaved. Let $\chi_z = 2\mu m_z/(8\pi^2 f^2)$, where z labels quark type ($z = x, y, q, s$). Then $\mathcal{O}(m^3)$ analytic corrections to decay constant are

$$\frac{f_\pi^{\rm NNLO}}{f} = \beta_1^{(f)}(\chi_x+\chi_y)^2 + \beta_2^{(f)}(2\chi_q+\chi_s)^2 + \beta_3^{(f)}(\chi_x+\chi_y)(2\chi_q+\chi_s) + \beta_4^{(f)}(\chi_x-\chi_y)^2 + \beta_5^{(f)}\left(2\chi_q^2+\chi_s^2\right)\,. \tag{8}$$

The interchange symmetries among valence quarks $x \leftrightarrow y$ and sea quarks $u \leftrightarrow d \leftrightarrow s \leftrightarrow u$ restrict the form of the terms.

There are 5 corresponding terms (with coefficients $\beta_1^{(m)}, \dots, \beta_5^{(m)}$) for the meson mass at NNLO.

Note that "chiral coupling," $1/(16\pi^2 f^2)$ in eqs. (6) and (7), is expressed in terms of bare (tree-level) parameter f. For better convergence of χPT, we believe one should put a *physical* parameter here: $f \to f_\pi$ or f_K. (This is like argument for using physical "boosted" coupling in ordinary perturbation theory.) The difference is a NNLO effect. In practice, try 3 approaches:

(1) Leave coupling as $1/(16\pi^2 f^2)$
(2) Fix coupling as $1/(16\pi^2 f_\pi^2)$
(3) Write coupling as $\omega/(16\pi^2 f_\pi^2)$ and allow ω to vary around 1 in fit, with standard deviation 0.1, using Baysean priors [11].

Choice (3) gave the best fits and is used for central values. Choice (2) gave acceptable fits and is used for systematic error estimates. Choice (1) did not give acceptable fits and is at present not included in the analysis. More study is probably warranted, however.

As test for convergence of χPT, a NNNLO term also included. We use

$$\frac{f_\pi^{\rm NNNLO}}{f} = \rho^{(f)}(\chi_x+\chi_y)^3 + \cdots\,, \tag{9}$$

with corresponding term with coefficient $\rho^{(m)}$ for the meson mass. Values of $\rho^{(f)}$ and $\rho^{(m)}$ from fits are $\lesssim 0.1$.

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Chiral Fits: Parameters

Inventory of fit parameters:

- Tree level
  2 unconstrained parameters: μ [eq. (6)] and f [eq. (7)].
- NLO physical parameters
  4 unconstrained parameters: $2L_8 - L_5$, $2L_6 - L_4$ [eq. (6)], L_5, L_4 [eq. (7)].
- NLO taste-violating [$\mathcal{O}(a^2)$] parameters
  4 unconstrained parameters: δ'_V, δ'_A, C [eq. (6)], F [eq. (7)].
- NNLO physical parameters
  10 constrained parameters: $\beta_1^{(m)}, \dots, \beta_5^{(m)}$ and $\beta_1^{(f)}, \dots, \beta_5^{(f)}$ [eq. (8)]; constrained with Baysean priors to have standard deviation of 1 around 0.
- NNNLO physical parameters
  2 constrained parameters: $\rho^{(m)}$ and $\rho^{(f)}$ [eq. (9)]; constrained to have standard deviation of 1 around 0.
- "Smoothed r_1" parameters
  4 constrained parameters: $C_0, \dots, C_3$ [eq. (2)]; allowed to vary by 1 standard deviation around central values of the r_1-smoothing fit.
- "Chiral coupling" parameter
  1 constrained parameter: in fits that give central values, ω is allowed to vary around 1 with standard deviation 0.1. In other fits ω is held fixed to 1.

So far, total number of parameters is 27 (or 26 with ω fixed): 19 (18) physical parameters, 4 taste-violating parameters, and 4 r_1-smoothing parameters.

Want to fit coarse and fine lattices simultaneously $\Rightarrow$ parameters must be allowed to change with a^2. Force taste-violating parameters to change by factor of 0.375 ($\approx$ ratio of $\alpha_S^2 a^2$).

When taste violations removed, residual errors are $\mathcal{O}(\alpha_S a^2)$. For physical parameters, expect value on coarse lattice to differ from that on fine lattice by $\alpha_S a^2 \Lambda^2_{QCD} \sim 2\%$.

Therefore also include:

- "Scaling" parameters
  19 (18) tightly constrained parameters: fractional difference between physical parameters on coarse and fine lattices. Constrained to be 0 with standard deviation of 0.02 to 0.025 in central value fits; this is changed to be 0.01 or 0.04 in fits used to estimate systematics.

Total is 46 (44) parameters, although most are constrained or tightly constrained.

Notes:

(1) Various meson masses entering NLO chiral logs are determined by tree-level fits (Fig. 2), and are **NOT** free parameters in chiral log fits.
(2) r_1-smoothing parameters and errors already come from fit to both coarse and smooth sets $\Rightarrow$ don't allow values to vary when going from coarse $\to$ smooth.
(3) If parameter δ'_A were negative and large compared to the splitting in the taste-axial channel, Δ_A,

$$\delta'_A < \delta'_{A,\,\rm crit} \equiv -4\Delta_A\,\frac{1 + a^2\Delta_A/(m_s^{\rm phys})^2}{2 + 3a^2\Delta_A/(m_s^{\rm phys})^2}\,, \tag{10}$$

$m^2_{\eta_A}$ would go to zero before $m_q \to 0$, and a transition to an unusual phase would occur (see C. Aubin's talk). This condition does *not* appear to be satisfied in practice, but a weaker condition that would allow a phase transition as all 3 quark masses get small appears more likely to be satisfied. The implications of such a phase transition are not understood.

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Chiral Fits: Data

Let P be a generic partially quenched pseudoscalar. Fit partially quenched data for $m_P^2/(m_x + m_y)$ and f_P simultaneously, with covariances, to above form.

Consider fits on two sets of data:

(A) Maximum quark mass of $\approx 0.8m_s^{\rm phys}$; 194 data points. Data set (A) $\Rightarrow$ central values of f_π, L_i, and $m_q^{\rm phys}$ (physical value of average u, d mass).

(B) Maximum quark mass of $\approx m_s^{\rm phys}$; 324 data points. Data set (B) $\Rightarrow$ central values of f_K, and $m_s^{\rm phys}$.

Alternative fit type and variation in restrictions on fit parameters $\Rightarrow$ estimate of systematic error.

For each chiral log fit, we quote two confidence levels (CLs). First is standard CL, with χ^2 summed over all data points, and ${\rm d.o.f} = \#\,{\rm data\ pts} - \#\,{\rm params}$. Second CL adds contributions of Baysean priors: each constraint on a fit parameter is treated as if it were an additional data point and contributes both to χ^2 and d.o.f.

Figures 3–5 show the results of two chiral fits. Figures 3 and 4 come from our *single*, central value fit on data set (A). Similarly, Fig. 5 comes from our central value fit on data set (B).

In all cases, we show for clarity only a small fraction of the data points in the fit. Figures 3 and 4 show "pion" points with $m_x = m_y$. Figure 5 shows "kaon" points with $m_y \approx m_s^{\rm phys}$.

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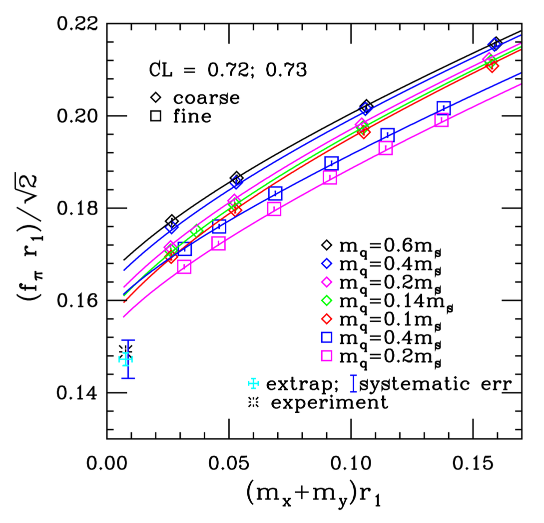
Figure 3



"Pion" decay constants with $m_x = m_y$. Lines come from *single* fit to entire data set (A). Points (and fit lines) have been corrected for finite volume effects using eq. (5). See below for description of how extrapolation was performed.

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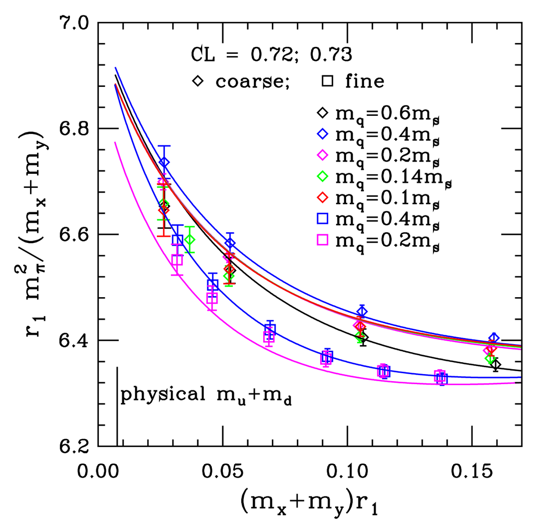
Figure 4



Same as Fig. 3, but for "pion" masses. Because taste splittings are smaller for the fine lattices, the average meson mass changes more rapidly with quark mass, and the rise at small quark mass is steeper.

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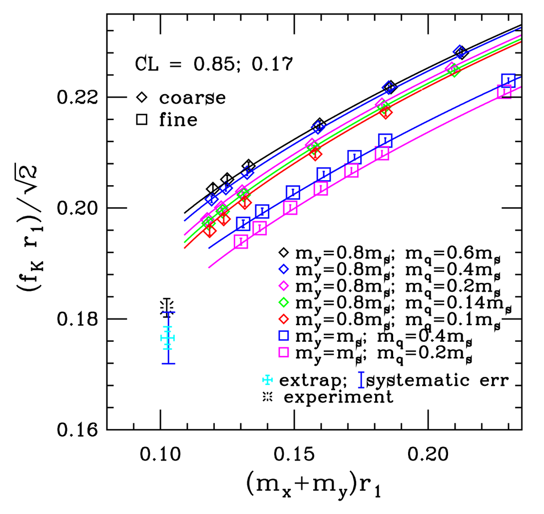
Figure 5



"Kaon" decay constants with m_y fixed as closely as possible on each set to $m_s^{\rm phys}$. Lines come from *single* fit to entire data set (B). Points (and fit lines) have been corrected for finite volume effects using eq. (5).

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Chiral Fits: Comments

- Fit to data set (A) (Figs. 3 and 4; valence masses $\lesssim 0.8\, m_s^{\rm phys}$) appears completely acceptable.
- Fit to set (B) (Fig. 5; valence masses $\lesssim m_s^{\rm phys}$) shows signs of χPT starting to break down. Some of the NNLO parameters are ~ 3 instead of $\lesssim 1$. This is reflected by second CL (0.17), which includes Baysean priors: priors are "unhappy" that some NNLO terms are rather large. Still, this fit is a good interpolation around $m_s^{\rm phys}$; use it for kaon physics, but not for determining f_π or L_i.
- Good fits **NOT** possible without the taste violating terms in SχPT. With continuum form (*i.e.*, without params δ'_V, δ'_A, C, and F, and with taste splittings set to zero), typical fits have CL $< 10^{-50}$.
- Continuum extrapolation: set $\mathcal{O}(a^2)$ params (δ'_V, δ'_A, C and F) to 0; extrapolate physical params linearly in $\alpha_S a^2$. Assuming $\alpha_S = \alpha_V(q^* = 3.33/a)$, $\alpha_S a^2$ changes by factor 0.428 going from coarse to fine. Final results not very sensitive to choice of q^* here or in assumed behavior of taste violations ($\alpha_S^2 a^2$). Variations in q^* included in systematic error estimates.
- Figure 6 shows behavior of f_π and f_K with $\alpha_S a^2$, before and after setting taste violations to 0. Once taste violations are removed, remaining discretization errors quite small: $\lesssim 1\%$ change between coarse and fine. This remains true even if requirement that physical fit params change by $\sim 2\%$ between coarse and fine is relaxed to $\sim 4\%$.

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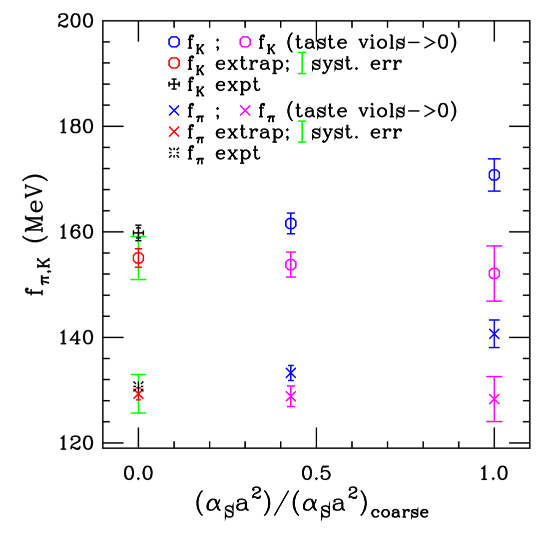
Figure 6



Dependence of chirally-extrapolated decay constants on lattice spacing.

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Results

- Preliminary results for decay constants:

$$\begin{aligned} f_\pi &= 129.3 \pm 1.1 \pm 3.5\ {\rm MeV} \\ f_K &= 155.0 \pm 1.8 \pm 3.7\ {\rm MeV} \\ f_K/f_\pi &= 1.201(8)(15)\,, \end{aligned} \tag{11}$$

where first error is statistical; second is systematic. Largest systematic error on f_π and f_K is 2.2% scale uncertainty. Chiral and continuum extrapolation errors estimated together: get 1 to 1.5% error by considering variations over alternative fits and variations in assumptions about a dependence.

The experimental numbers are: $f_\pi = 130.7 \pm 0.4$ MeV, $f_K = 159.8 \pm 1.5$ MeV, $f_K/f_\pi = 1.223(12)$.

- Preliminary results for Gasser-Leutwyler parameters at $\Lambda_\chi = m_\eta$:

$$\begin{aligned} 2L_6 - L_4 &= 0.5(2)\left({}^{+1}_{-3}\right) \times 10^{-3} \\ 2L_8 - L_5 &= -0.1(1)\left({}^{+1}_{-3}\right) \times 10^{-3} \\ L_4 &= 0.3(3)\left({}^{+7}_{-2}\right) \times 10^{-3} \\ L_5 &= 1.9(3)\left({}^{+6}_{-2}\right) \times 10^{-3}\,, \end{aligned} \tag{12}$$

Systematic errors here dominated by differences over acceptable fits. At present, make conservative choice and include fits to data set (B) in this estimate. Restriction to data set (A) makes many error estimates significantly smaller.

Continuum estimates for L_i [12] are $L_5 = 2.3(2)\times 10^{-3}$; $L_4 \approx L_6 \approx 0$.

[Comparisons between different estimates of L_i are, however, somewhat delicate, since they can depend significantly on treatment of NNLO terms.]

Result for $2L_8 - L_5$ is well outside the range that allows for $m_u = 0$ [13]:

$$-3.4\times 10^{-3} \lesssim 2L_8 - L_5 \lesssim -1.8\times 10^{-3}\,. \tag{13}$$

If preliminary result holds up, it would rule out $m_u = 0$ solution of the strong CP problem.

- Preliminary results for quark masses at scale 2 GeV:

$$\begin{aligned} m_s^{\overline{MS}} &= 70(15)\ {\rm MeV} \\ \hat m^{\overline{MS}} &= 2.7(6)\ {\rm MeV}\,, \end{aligned} \tag{14}$$

where $\hat m$ is the average of the u and d masses. Have used 1-loop perturbative results for the mass renormalization [14, 15]. Error is dominated by the $\mathcal{O}(\alpha_S^2)$ correction to the renormalization constant, estimated to be $\sim 20\%$ [14]. These quark masses are low compared to sum rule estimates [16]; but probably not inconsistent within errors of both approaches.

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