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# Some results from full 2+1 flavor simulations of QCD

Urs M. Heller

American Physical Society & BNL

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# Collaborators



MILC Collaboration (Jan 2004): E. Gregory, C. Aubin, R. Sugar, UMH, J. Hetrick, S. Gottlieb, C. Bernard, C. DeTar, J. Osborn, D. Toussaint

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+ **Fermilab, HPQCD & UKQCD Collaborations:**

C. Davies, M. Di Pierro, A.X. El-Khadra, E.D. Freeland, A. Gray, J. Hein, A.S. Kronfeld, G.P. Lepage, P.B. Mackenzie, Q. Mason, D. Menscher, M. Nobes, M. Okamoto, J. Shigemitsu, J. Simone, H. Trottier, M. Wingate

# Outline

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- Simulation Choices & Ensemble of Configurations
- Result Highlights/Summary
- Pseudoscalar decay constants, quark masses, etc.
- Baryons
- Heavy-light decay constants
- Semileptonic B/D decays
- Summary and Outlook

# Simulation Choices

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To carry out a simulation we must select certain physical parameters:

- lattice spacing ( $a$ ) or gauge coupling ( $\beta$ )
- grid size ( $N_s^3 \times N_t$ )
- quark masses ( $m_{u,d} = m_l, m_s$ )

To control systematic error we must

- take continuum limit,  $a \rightarrow 0$
- take infinite volume limit
- extrapolate to physical light quark mass;  
we can work at physical  $s$  quark mass, or interpolate to it

# Simulation Choices

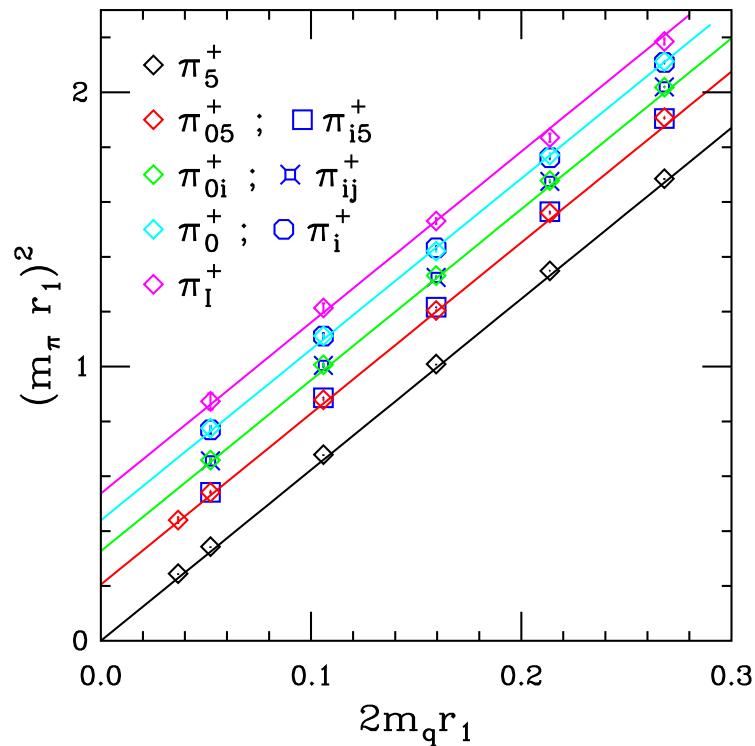
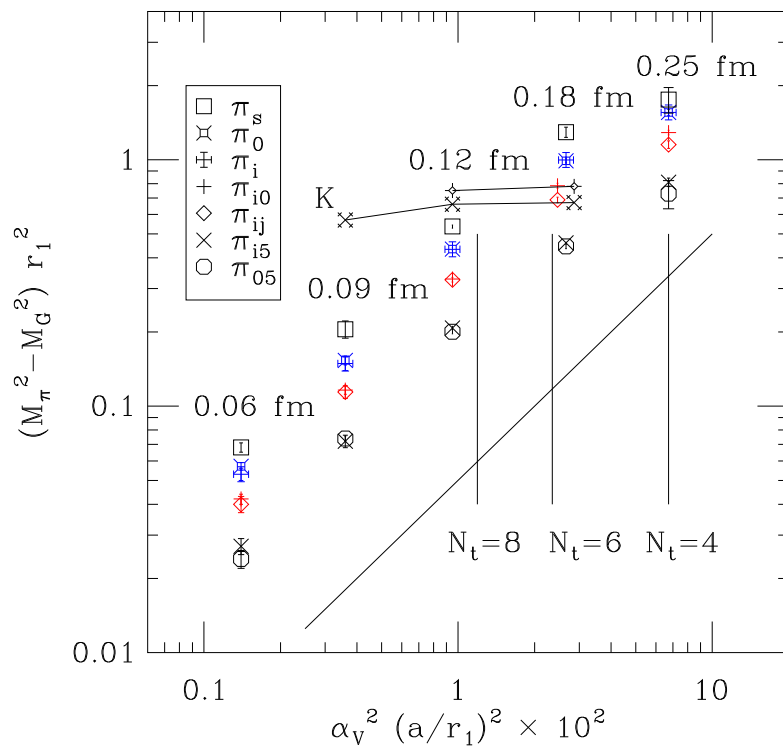
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We also must choose an action and a simulation algorithm.

- The gauge action is a 1-loop improved Lüscher-Weisz action, with  $\mathcal{O}(\alpha_s^2 a^2)$  discretization errors.
- The fermion action is a tree-level improved staggered action with a “fat” link to suppress taste violations of the staggered fermions. It has  $\mathcal{O}(\alpha_s a^2)$  discretization errors.
- The algorithm is the Hybrid Molecular Dynamics R-algorithm, with the  $\det^{1/4}$  trick to eliminate the extra tastes.
- Recently, switched to exact RHMC algorithm

Whether the  $\det^{1/4}$  trick induces **non-localities** in the **interacting** theory is an open question. Our results, so far, show **no sign of a problem**.

# Taste violations



The taste splittings are independent of  $m_q$ , and **vanish in the continuum limit, as expected, i.e. as  $\alpha_s^2 a^2$ .**

This is consistent with  $\det D_{stag} \rightarrow (\det D_{1f})^4$  as  $a \rightarrow 0$ .

# Ensemble of Configurations

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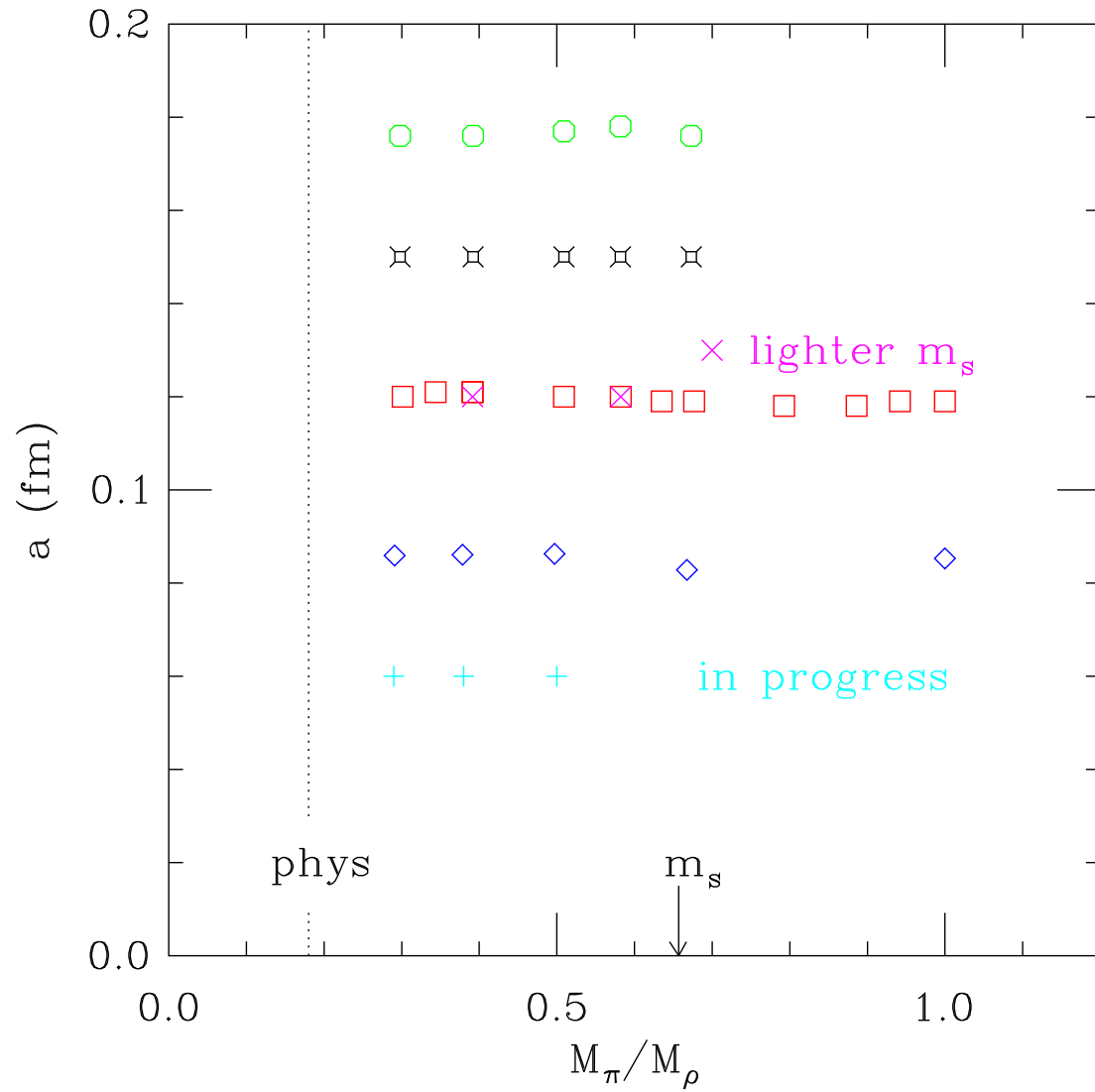
MILC has been generating three flavor configurations to allow control of these errors:

- most results are based on three lattice spacings, 0.121 fm, 0.086 fm, and 0.06 fm, kept fixed for different quark masses; some use also 0.176 fm and  $\sim 0.15$  fm.
- mostly  $V_s \sim (2.4 \text{ fm})^3$ , with one  $\sim (3.4 \text{ fm})^3$ , to check for finite volume effects; except 1 set:  $m_\pi L > 4$ .
- several  $m_{u,d} = \hat{m}'$  to extrapolate to physical light quarks; use two  $m'_s$  (at  $a = 0.12$  fm) to interpolate to physical strange quark mass

The ensembles of configurations are available to others through the NERSC Gauge Connection.

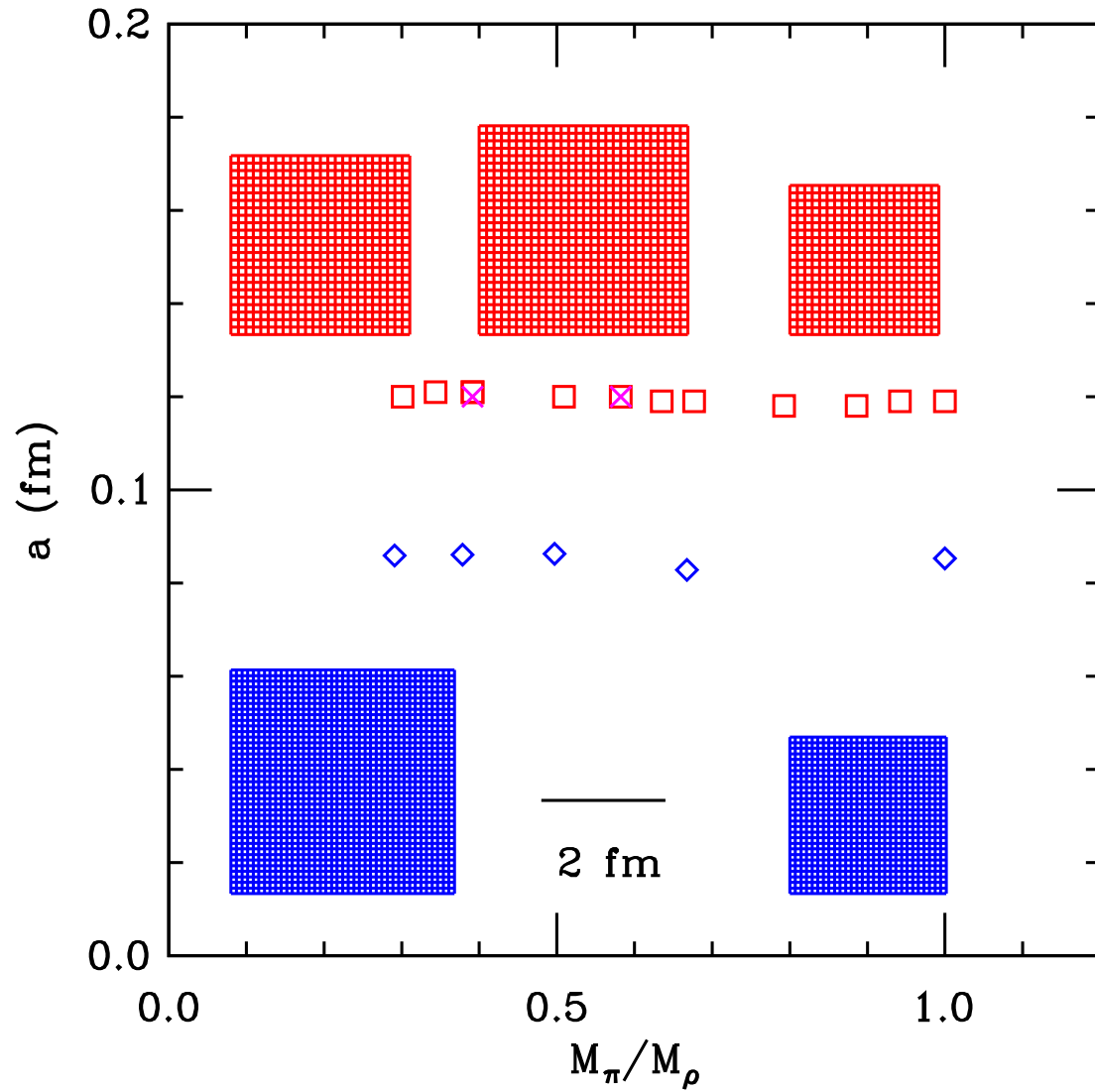
Some new configurations generated with USQCD resources.

# MILC Ensembles

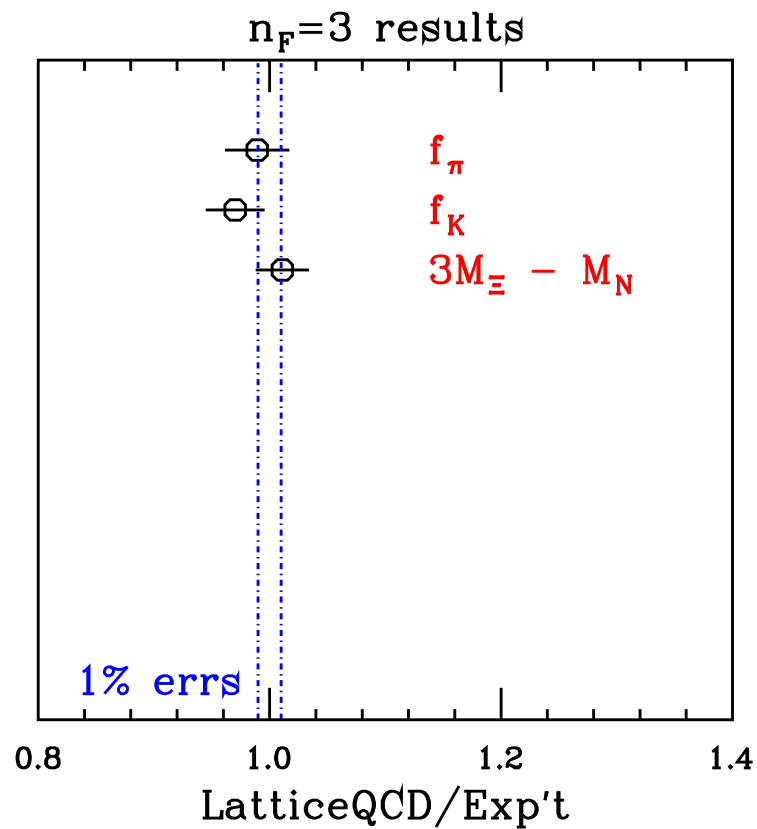
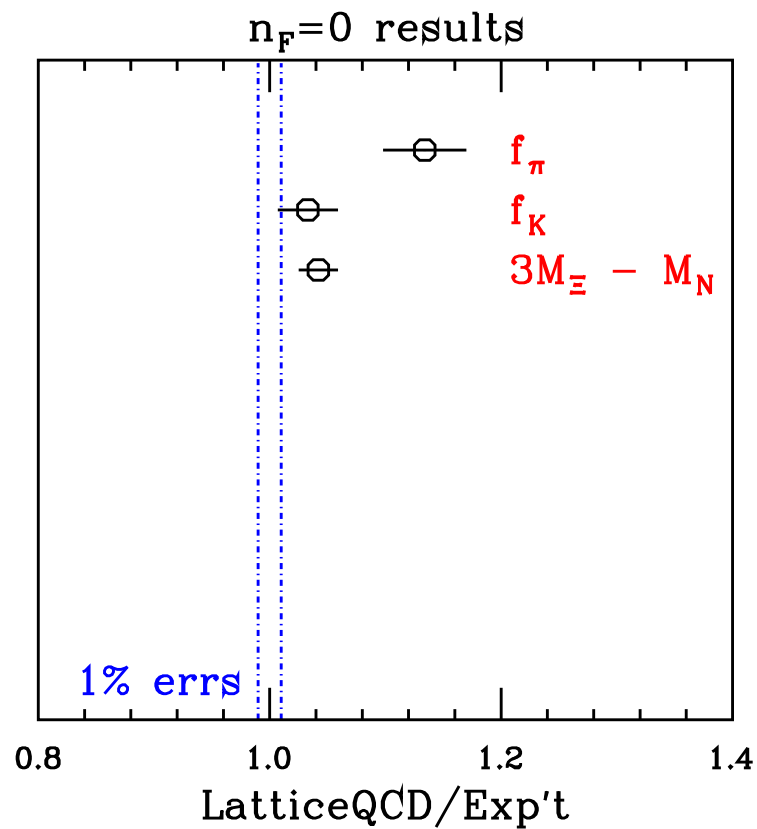




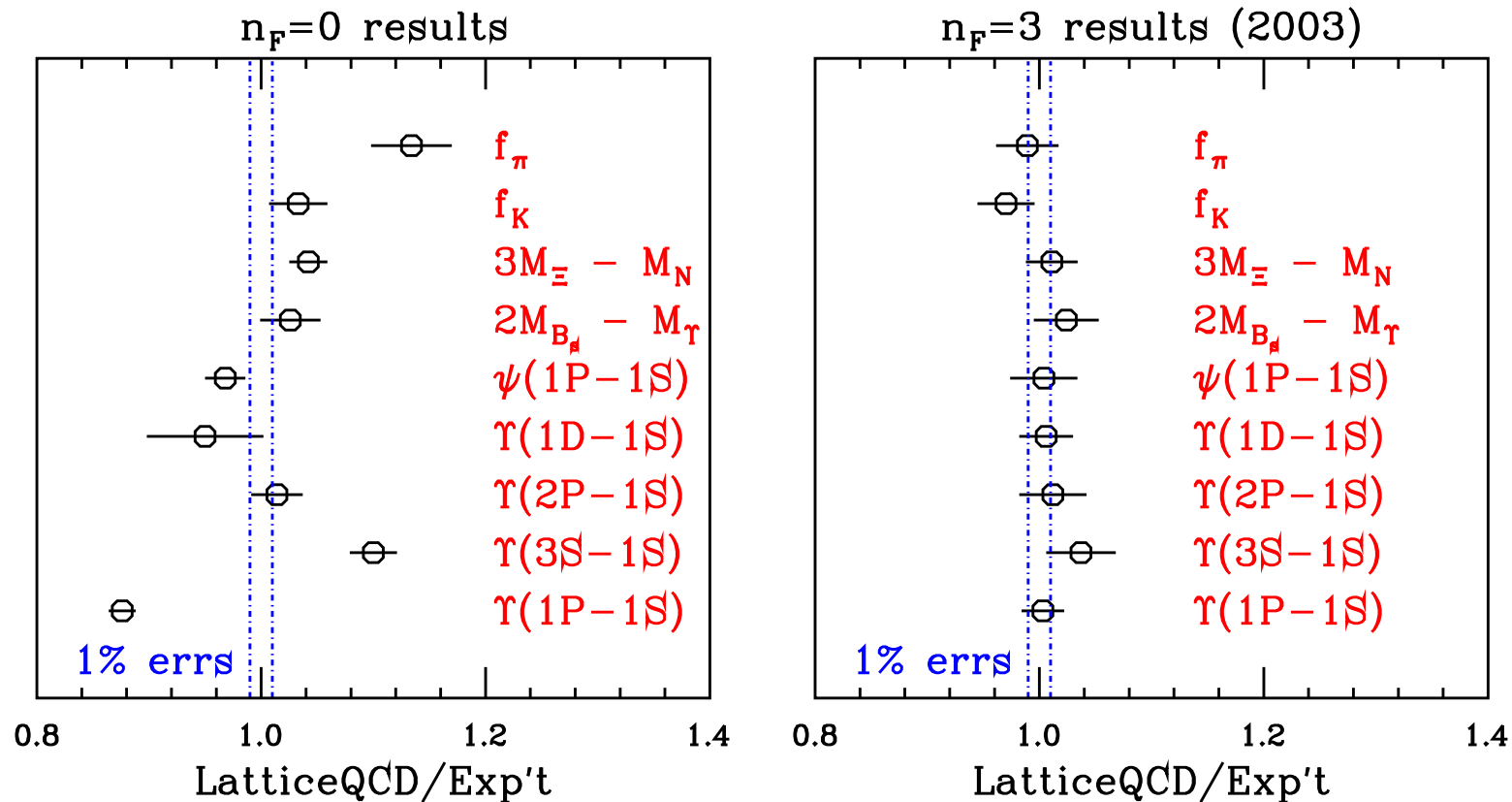
# MILC Ensembles



# Ratio Plot



# Ratio Plot



By sharing with FNAL, HPQCD and UKQCD:

C.T.H. Davies *et al.*, PRL 92 (2004) 022001 [hep-lat/0304004]

# Chiral perturbation theory ( $\chi$ PT)

For extrapolation in quark mass use chiral perturbation theory ( $\chi$ PT), an **effective field theory** based on **symmetry** considerations – and its breaking:

$$\mathcal{L}_{\chi PT} = \frac{f^2}{8} \text{Tr} \left( \partial_\mu \Sigma \partial_\mu \Sigma^\dagger \right) - \frac{1}{4} \mu f^2 \text{Tr} \left( \mathcal{M} \Sigma + \mathcal{M} \Sigma^\dagger \right) + \mathcal{O}(p^4, mp^2, m^2),$$

where  $\Sigma = \exp(i\phi_a t_a / f)$  ( $\phi_a = \pi^0, \pi^\pm, K^0, \bar{K}^0, K^\pm, \eta$ ). One finds,

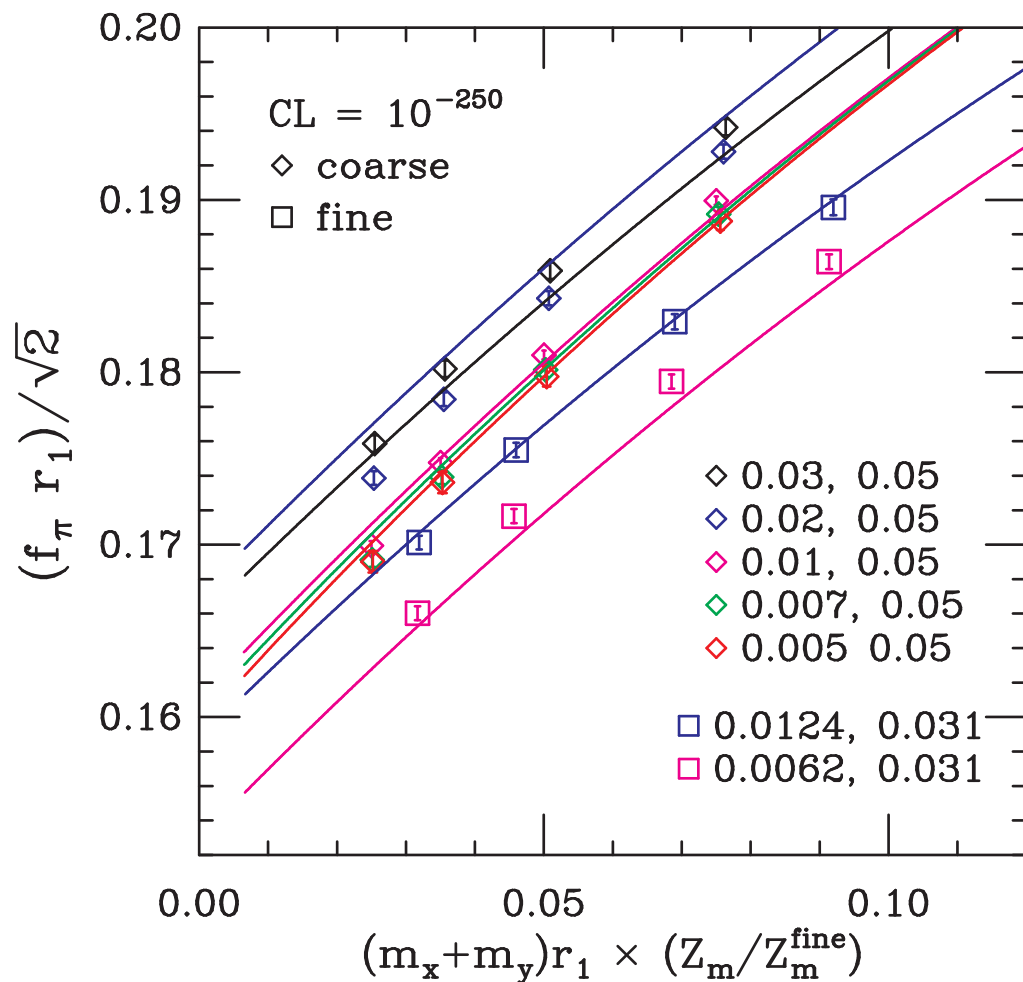
$$\frac{m_\pi^2}{2m_q} = \mu \left\{ 1 + \frac{1}{16\pi^2 f^2} \left[ \frac{2}{3} (2\mu m_q) \log \left( \frac{2\mu m_q}{\Lambda^2} \right) + \text{''}p^4 - \text{terms''} \right] \right\},$$
$$f_\pi = f \left\{ 1 + \frac{1}{16\pi^2 f^2} \left[ -3(2\mu m_q) \log \left( \frac{2\mu m_q}{\Lambda^2} \right) + \text{''}p^4 - \text{terms''} \right] \right\},$$

for 3 degenerate flavors. The **low energy parameters** ( $f, \mu, \dots$ ) are to be determined from the **lattice simulations**.

# Light pseudoscalar sector

Have precise measurements for mass and decay constants

- Continuum  $\chi$ PT fit to both  $f_\pi$  and  $m_\pi$  at  $a = 0.12$  and  $0.09$  fm simultaneously
- Does not work:  $CL = 10^{-250}$
- Could first extrapolate to continuum and then make  $\chi$ PT fit; but loose information



# Staggered chiral perturbation theory (S $\chi$ PT)

Extend the effective field theory concept to include symmetry breaking terms particular to the **staggered lattice regularization**:

$$\mathcal{L}_{S\chi PT} = \mathcal{L}_{\chi PT} + a^2 \mathcal{V} .$$

Because of the four-fold doubling, each meson field has now 15 partners, e.g.  $\pi^+ \rightarrow \pi_A^+$ ,  $A = 1, \dots, 16$ . At tree level, the new term parametrizes the **taste symmetry breaking**,

$$m_{\pi_A}^{(0)2} = 2\mu m_q + a^2 \Delta_A .$$

At 1-loop, this **softens** the chiral logs, generically as

$$2\mu m_q \log(2\mu m_q / \Lambda^2) \rightarrow \frac{1}{16} \sum_A m_{\pi_A}^{(0)2} \log(m_{\pi_A}^{(0)2} / \Lambda^2) .$$

# Improved fits

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We can do better:

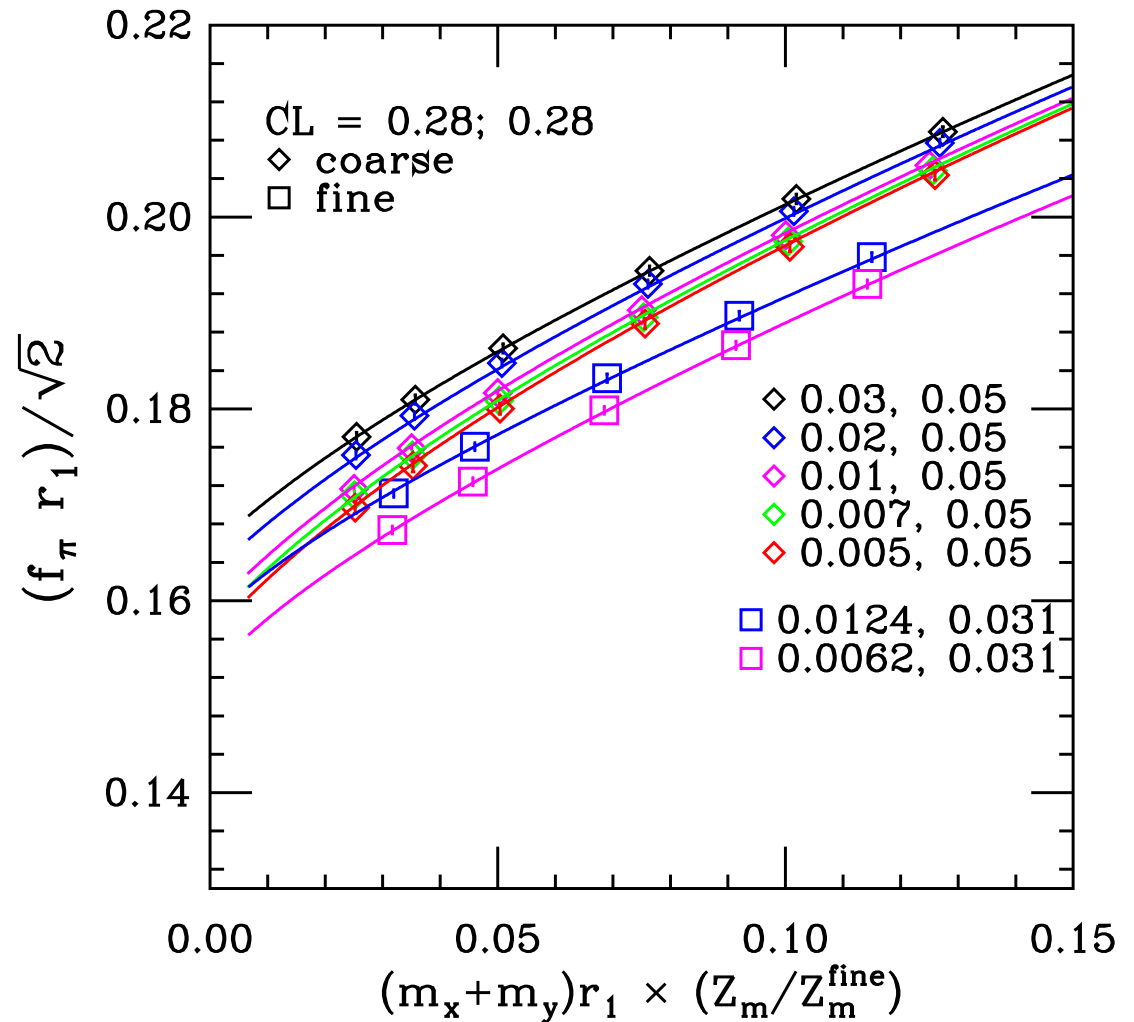
- use **S $\chi$ PT** (Aubin & Bernard), *i.e.* with taste violation  $\mathcal{O}(a^2)$  effects; include NNLO and NNNLO corrections
- fit coarse and fine lattices together: allow  $\mathcal{O}(a^2)$  corrections to physical  $\chi$ PT parameters
- apply finite volume corrections from finite volume  $\chi$ PT

After fit, we:

- extrapolate fit parameters to continuum
- show difference between  $m'_s$  (simulation strange mass) and  $m_s$  (correct value)
- see C. Aubin *et al.*, PRD 70 (2004) 114501 [hep-lat/0407028]
- major differences: (i) Second  $m'_s$  on coarse lattice. (ii) Lower  $m_l$  on fine lattice. (iii) Finer lattice with  $a = 0.06$  fm.

# Fit of $f_\pi$

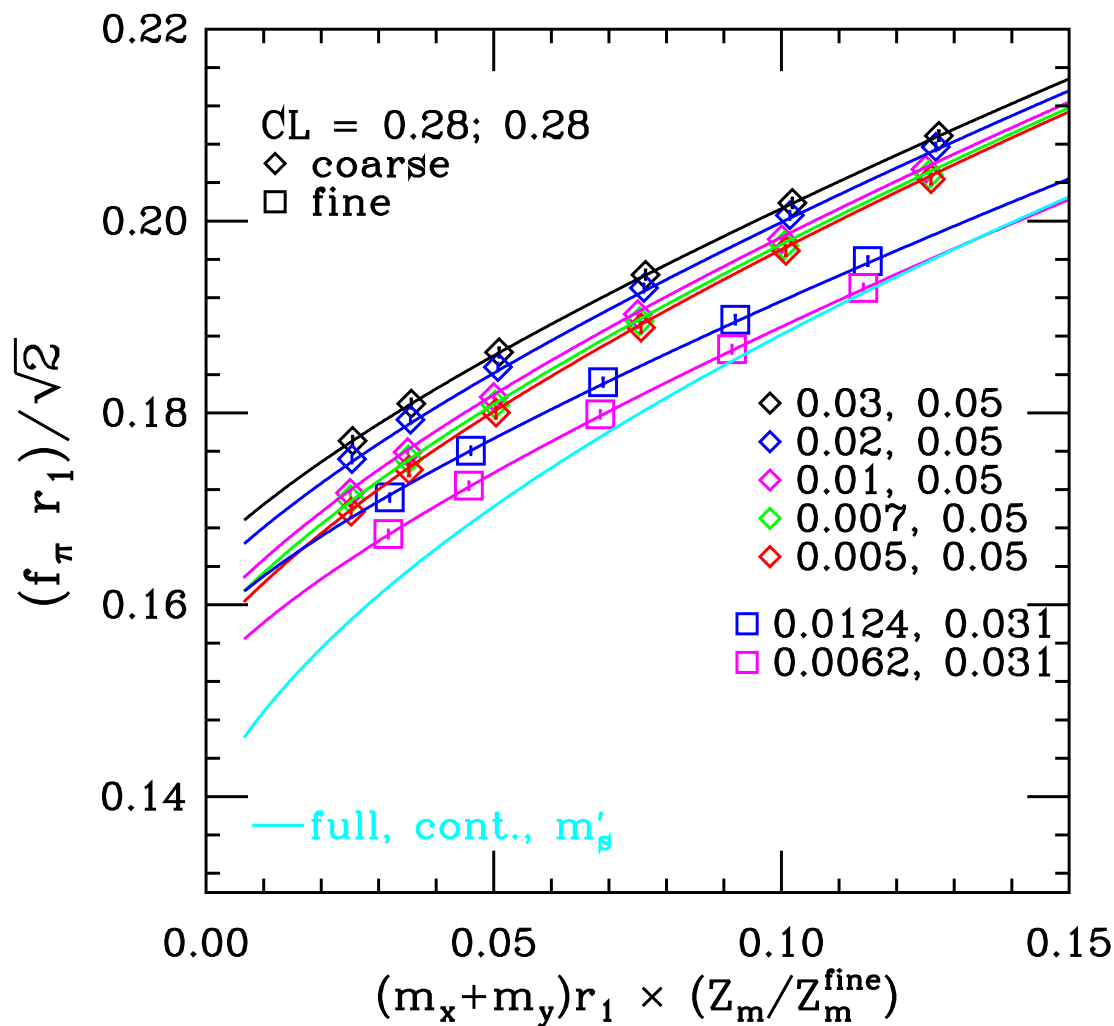
- Fit partially quenched  $f_\pi$  (and, simultaneously,  $m_\pi$ ) with taste violation terms and  $\mathcal{O}(a^2)$  corrections to physical  $\chi$ PT parameters





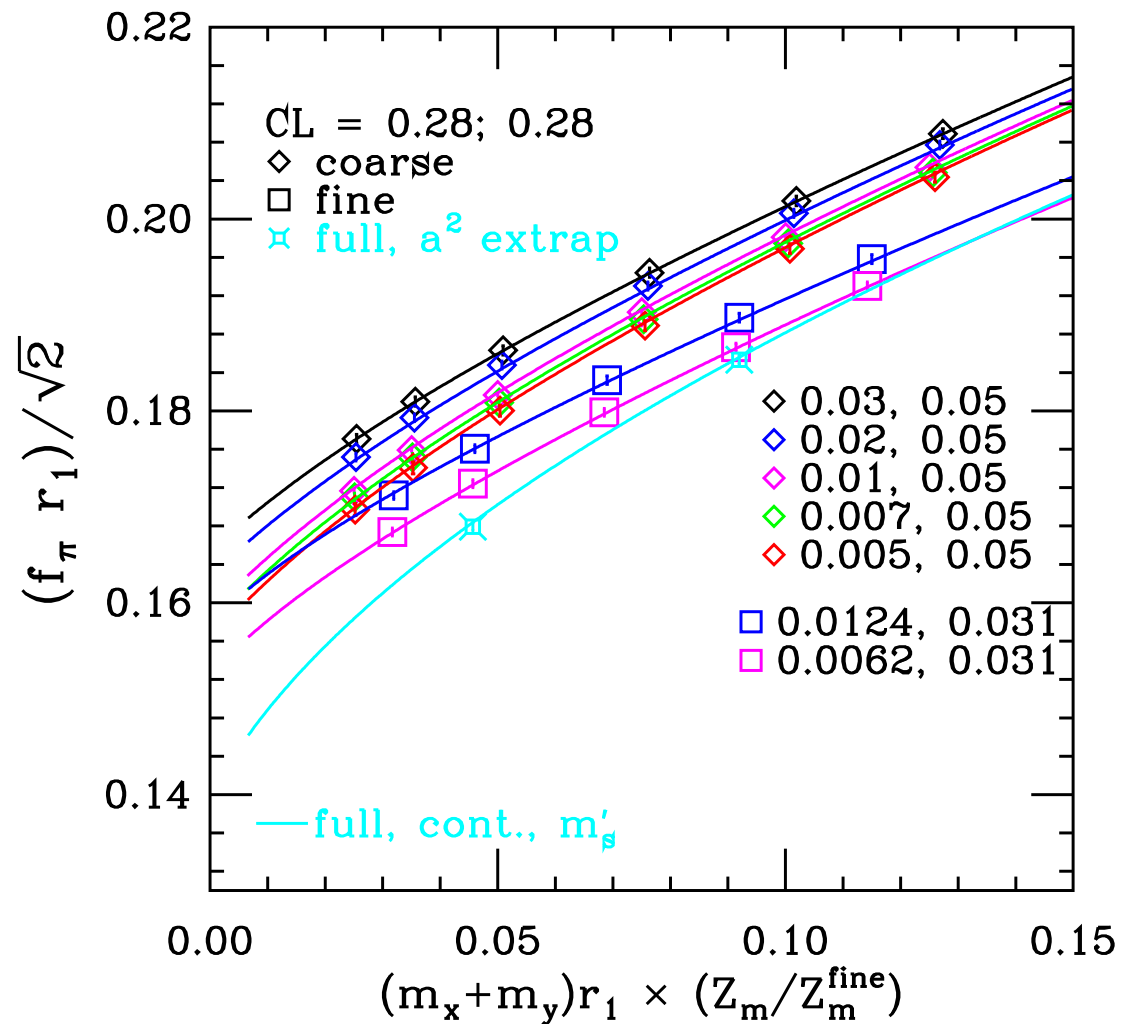
# Fit of $f_\pi$

- Extrapolate fit params to **continuum**, i.e., set  $\mathcal{O}(a^2)$  terms to zero
- Go to “**full QCD**:”  
Set  $\hat{m}'_{sea} = \hat{m}'_{val}$  and plot as function of  $\hat{m}'_{val}$ :



# Fit of $f_\pi$

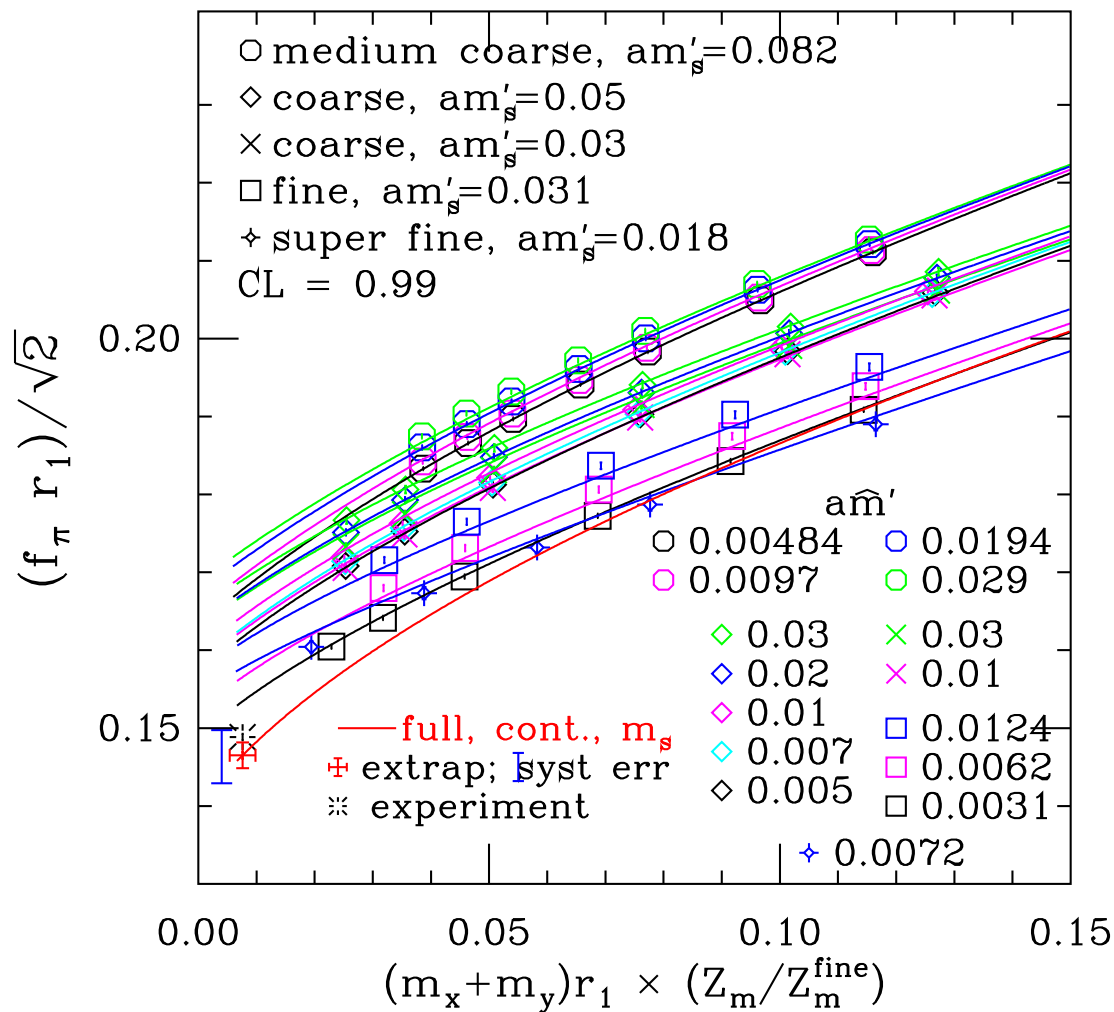
- Consistency check: extrapolate points with sea masses = valence masses to continuum at fixed quark mass



# Fit of $f_\pi$

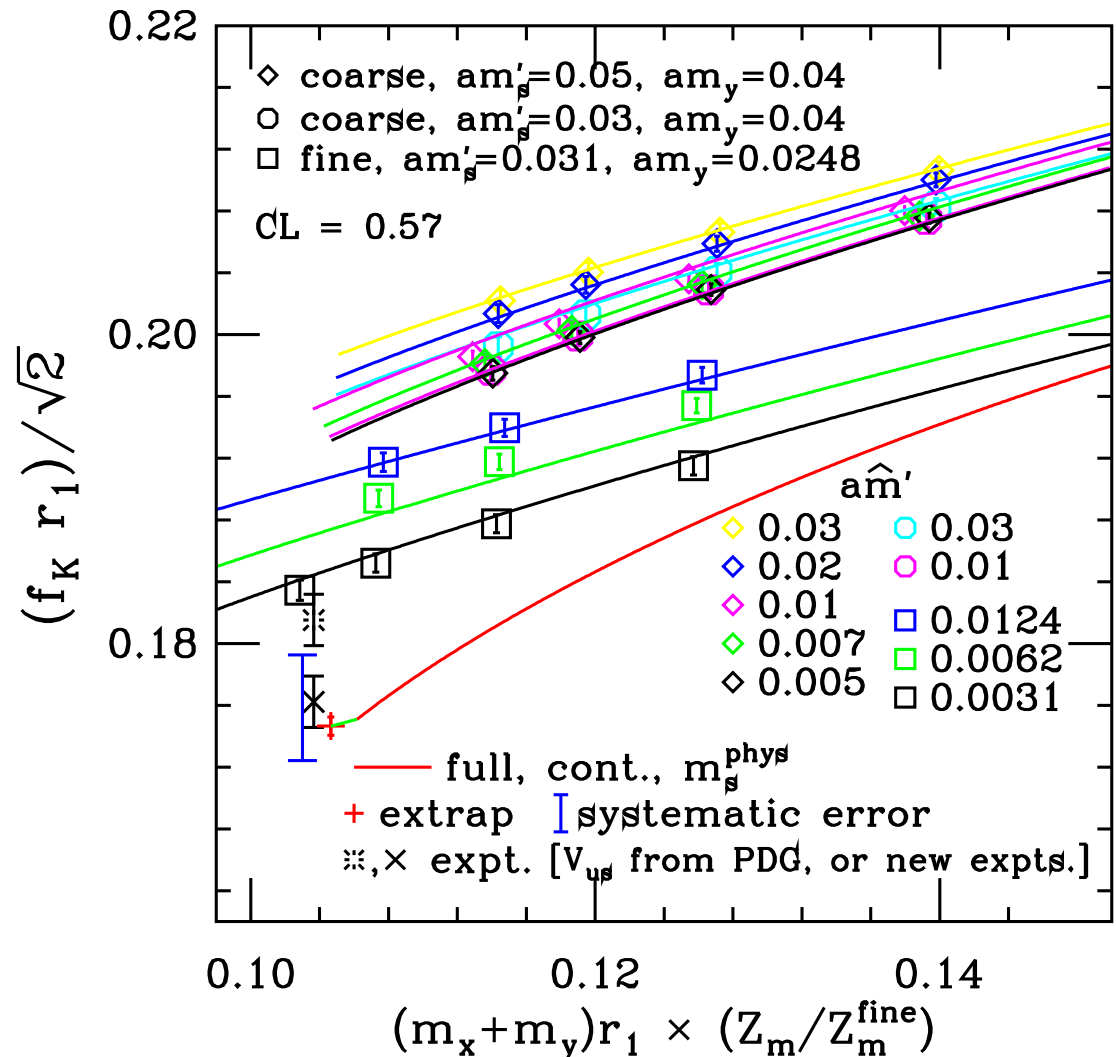
- Correct/interpolate from simulation strange mass,  $m'_s$ , to physical value,  $m_s$

In this last plot, data from second  $m'_s$  at  $a = 0.12$  fm, all data from  $a = 0.09$  fm, and first data from  $a = 0.06$  fm where included.

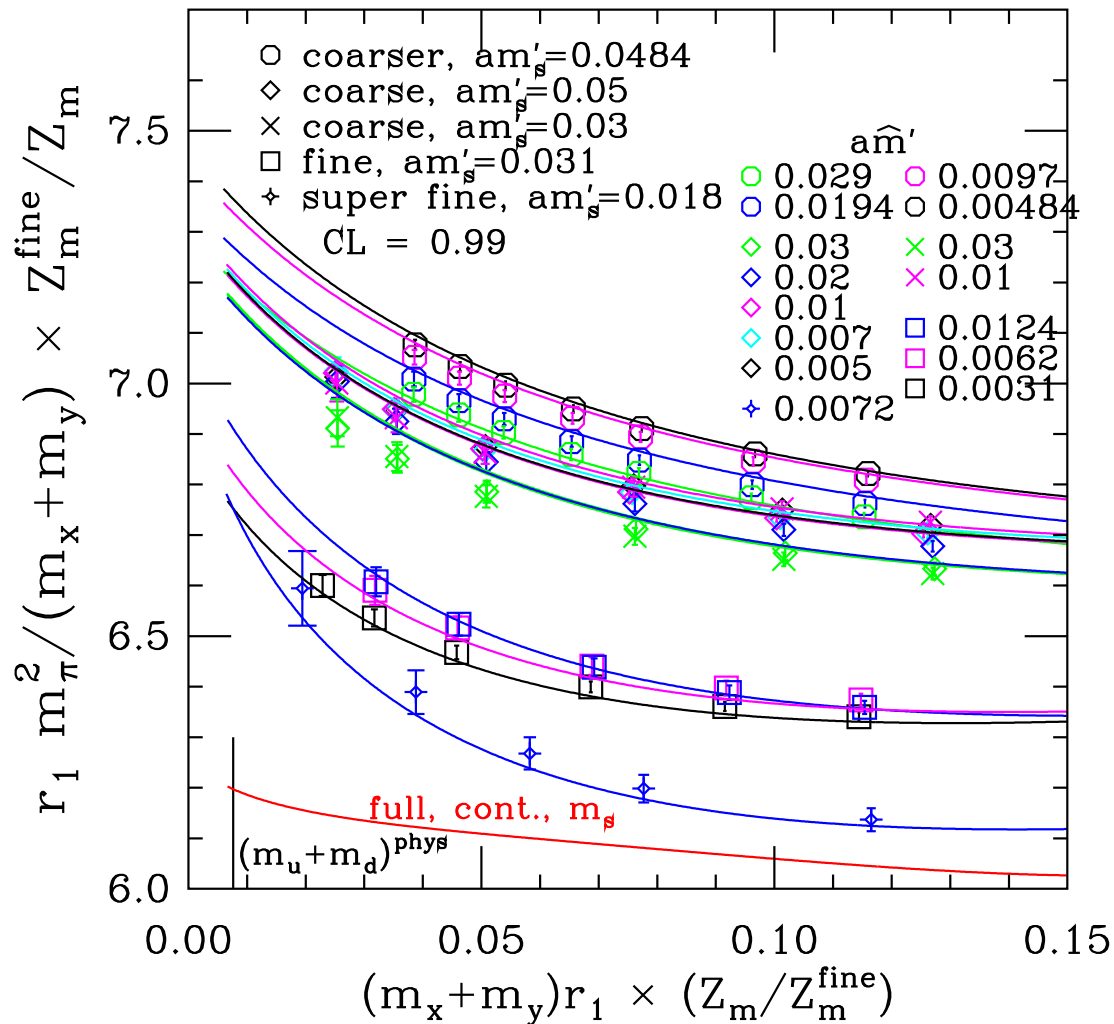


# Fit of $f_K$

- Similar procedure for  $f_K$ .
- But note that  $f_K$  is the decay constant of  $K^+$
- Here we need to extrapolate light valence quark to  $m_u$ , but light sea quark to  $\hat{m}$



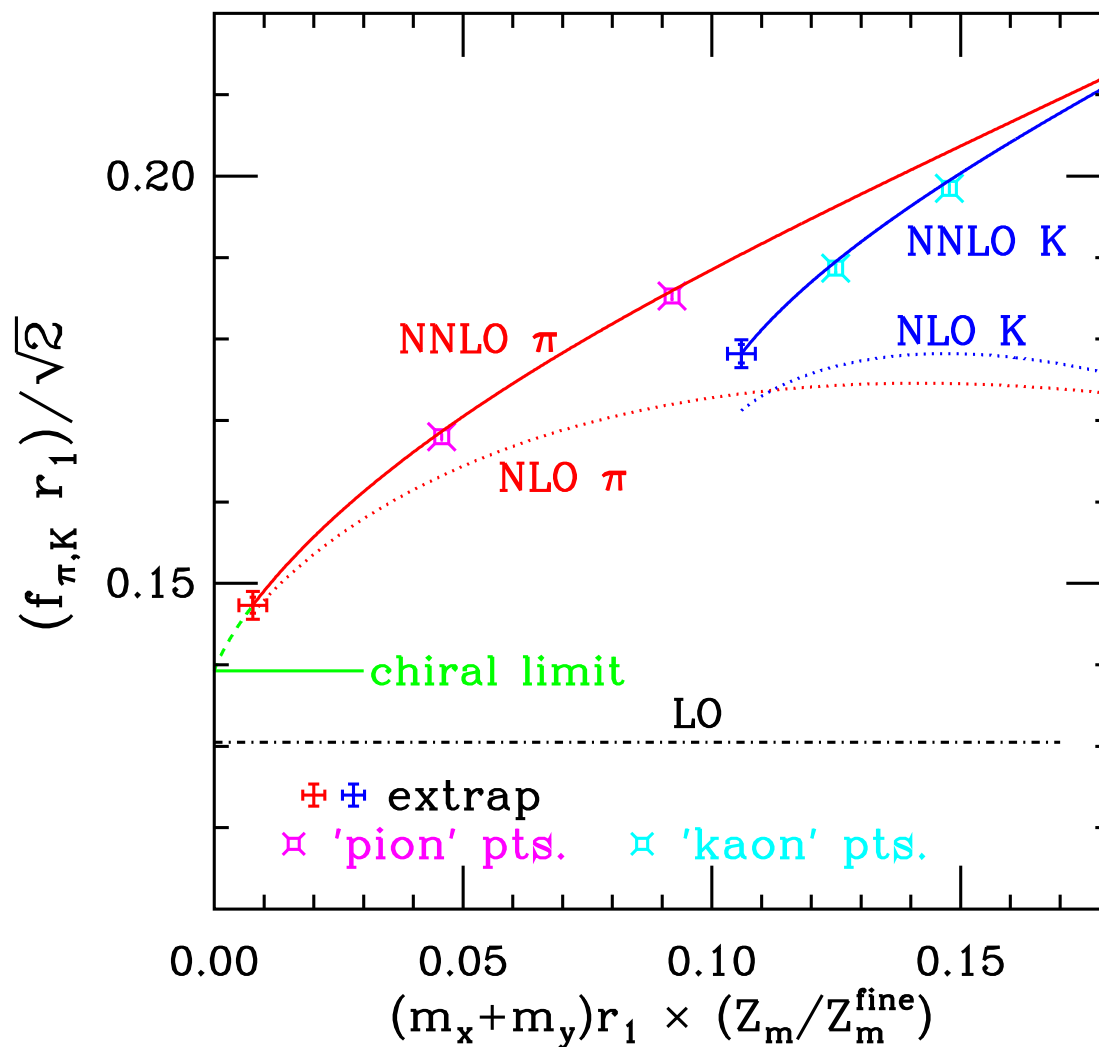
# Fit of $m_\pi^2 / (m_x + m_y)$



# Convergence of $SU(3)_L \times SU(3)_R$ $\chi$ PT

2004 fit:

*i.e.* no NNNLO terms



# Light Quark Masses

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To find quark masses, must extrapolate to the physical meson masses. Electromagnetic and isospin-violating effects are important

- Experimental masses:

$$m_{\pi^0}^{\text{expt}}, m_{\pi^+}^{\text{expt}}, m_{K^0}^{\text{expt}}, m_{K^+}^{\text{expt}}$$

- Masses with EM effects turned off:

$$m_{\pi^0}^{\text{QCD}}, m_{\pi^+}^{\text{QCD}}, m_{K^0}^{\text{QCD}}, m_{K^+}^{\text{QCD}}$$

- Masses with EM effects turned off and  $m_u = m_d = \hat{m}$ :

$$m_{\hat{\pi}}, m_{\hat{K}}$$

# EM & Isospin Violation

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$$m_{\hat{\pi}}^2 \approx (m_{\pi^0}^{\text{QCD}})^2 \approx (m_{\pi^0}^{\text{expt}})^2$$

$$m_{\hat{K}}^2 \approx \frac{(m_{K^0}^{\text{QCD}})^2 + (m_{K^+}^{\text{QCD}})^2}{2}$$

$$(m_{K^0}^{\text{QCD}})^2 \approx (m_{K^0}^{\text{expt}})^2$$

$$(m_{K^+}^{\text{QCD}})^2 \approx (m_{K^+}^{\text{expt}})^2 - (1 + \Delta_E) \left( (m_{\pi^+}^{\text{expt}})^2 - (m_{\pi^0}^{\text{expt}})^2 \right)$$

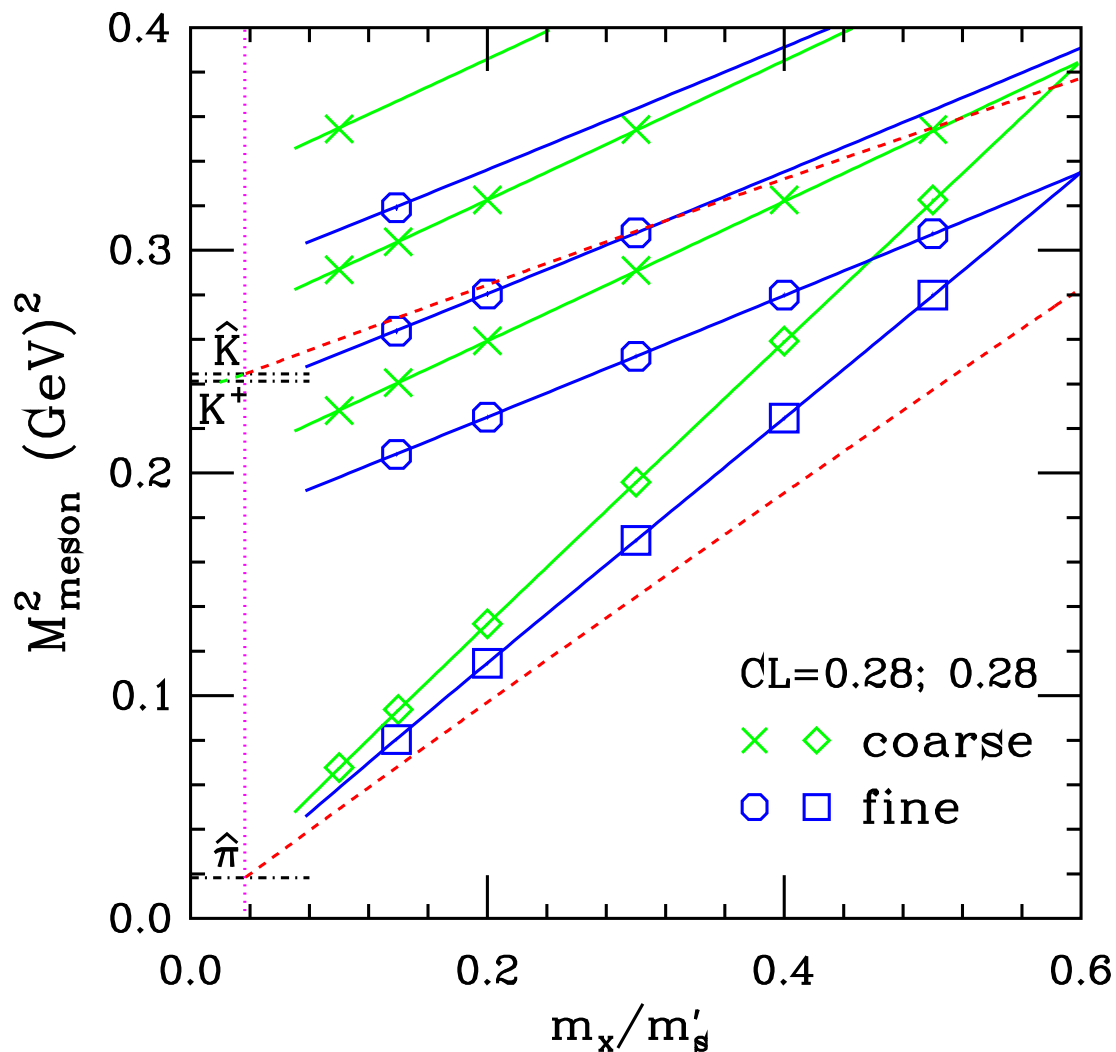
- $\Delta_E = 0$  is “Dashen’s theorem.”
- Continuum suggests:  $\Delta_E \approx 1$ .
- We use  $0 < \Delta_E < 2$



# Finding $\hat{m}$ , $m_s$

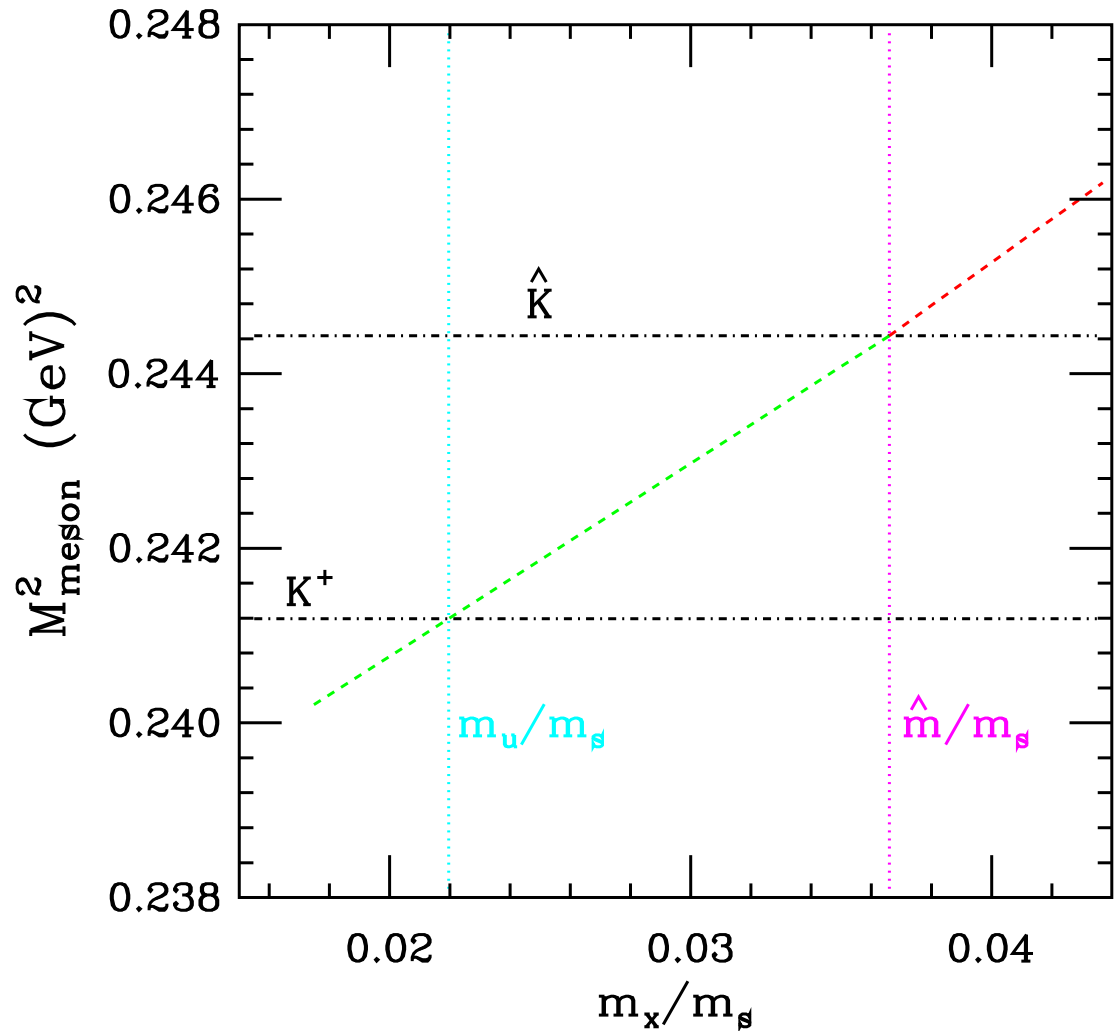
From 2004 fits.

- Subset of data with fits
- **Red lines** are continuum extrapolated full QCD fits with  $m_s$  **adjusted** so that both  $\hat{\pi}$  and  $\hat{K}$  are fit



# Finding $m_u$

- Next estimate  $m_u$  by extrapolating in quark mass to  $K^+$  mass
- Below  $\hat{m}$  only valence mass changes
- There is a small isospin violation because for sea quarks  $m_u = m_d = \hat{m}$



# Quark mass results

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We find

$$m_u/m_d = 0.42(0)(1)(4) ,$$

where the errors are statistical (rounded down to 0), lattice systematics, and a conservative estimate of EM effects.

Using instead a phenomenological result of Bijnens and Prades, NPB 490 (1997) 239 [hep-ph/9610360],  $\Delta_E = 0.84 \pm 0.25$ , we would obtain

$$m_u/m_d = 0.43(0)(1)(2) .$$

# Quark mass results

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Using a recent 2-loop mass renormalization constant (HPQCD collaboration, Q.Mason *et al.*, PRD 73 (2006) 114501 [hep-ph/0511160]) we obtain

$$\begin{aligned}m_s^{\overline{\text{MS}}} &= 90(0)(5)(4)(0) \text{ MeV} , \\ \hat{m}^{\overline{\text{MS}}} &= 3.3(0)(2)(2)(0) \text{ MeV} , \\ m_s/\hat{m} &= 27.2(0)(4)(0)(0) ,\end{aligned}$$

where the errors are from statistics, simulation systematics, perturbation theory ( $2\alpha^3$ ), and electromagnetic effects, respectively. The renormalization scale of the masses is 2 GeV. With  $m_u/m_d$  from above, then:

$$\begin{aligned}m_u^{\overline{\text{MS}}} &= 2.0(0)(1)(1)(1) \text{ MeV} , \\ m_d^{\overline{\text{MS}}} &= 4.6(0)(2)(2)(1) \text{ MeV} .\end{aligned}$$

# Results for light decay constants

We find (from preliminary 2005 fits):

$$\begin{aligned}f_{\pi} &= 128.6 \pm 0.4 \pm 3.0 \text{ MeV} , \\f_K &= 155.3 \pm 0.4 \pm 3.1 \text{ MeV} , \\f_K/f_{\pi} &= 1.208(2) \left( \begin{smallmatrix} +7 \\ -14 \end{smallmatrix} \right) .\end{aligned}$$

Experiments:

$$f_{\pi} = 130.7 \pm 0.4 \text{ MeV}, f_K = 159.8 \pm 1.5 \text{ MeV}, f_K/f_{\pi} = 1.223(12).$$

- Using our  $f_K/f_{\pi}$ , the experimental  $B(K \rightarrow \ell\nu)/B(\pi \rightarrow \ell\nu)$  and the well known Cabibbo angle  $V_{ud}$ :  $\Rightarrow V_{us} = 0.2223 \left( \begin{smallmatrix} +26 \\ -14 \end{smallmatrix} \right)$
- PDG (2006) value:  $V_{us} = 0.2257(21)$

# Results: Low Energy Constants

Also get (in units of  $10^{-3}$ , at chiral scale  $m_\eta$ ; 2004 fits):

$$2L_6 - L_4 = 0.5(1)(2) ,$$

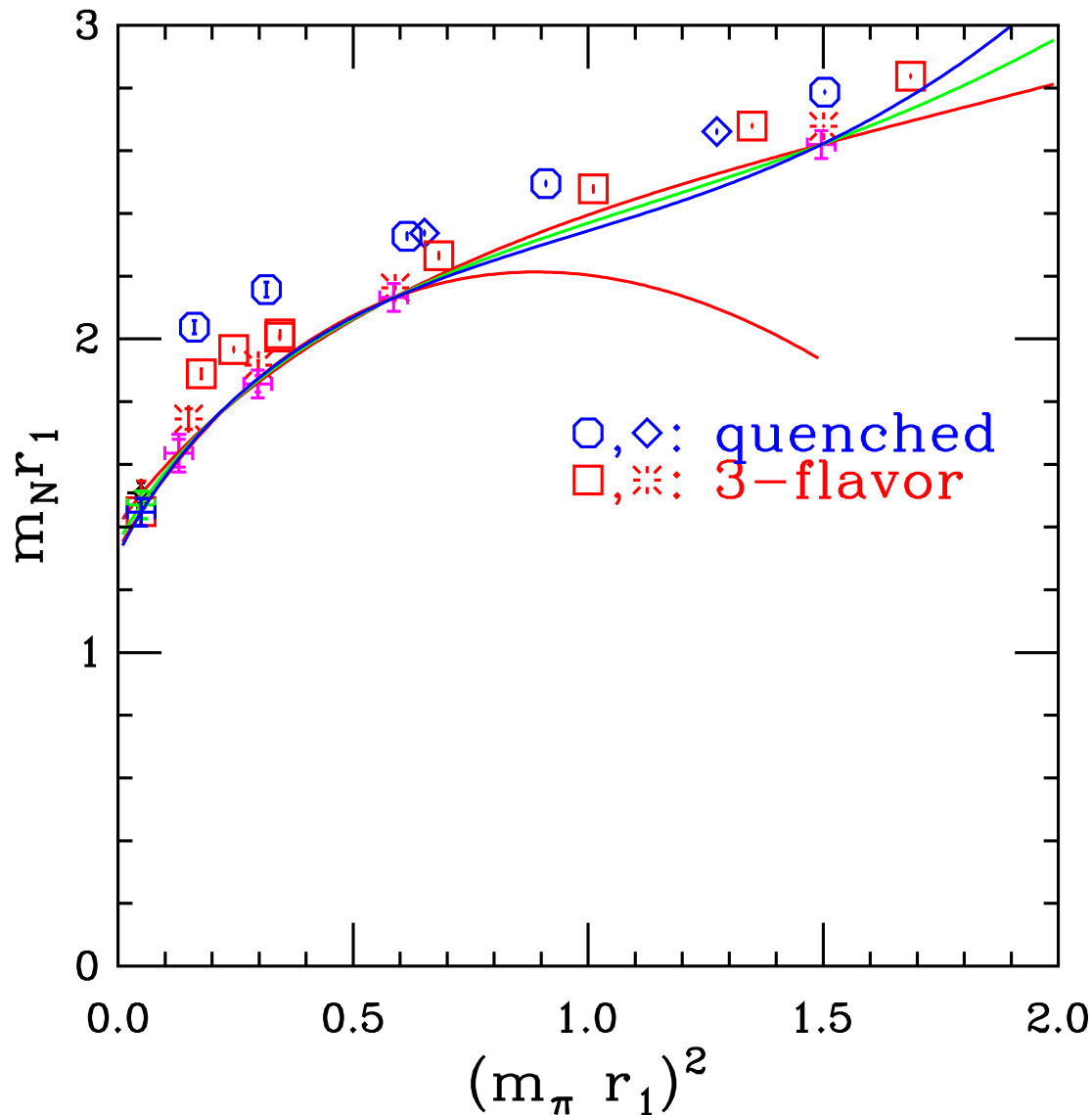
$$2L_8 - L_5 = -0.1(1)(1) ,$$

$$L_4 = 0.1(2)(2) ,$$

$$L_5 = 2.0(3)(2) .$$

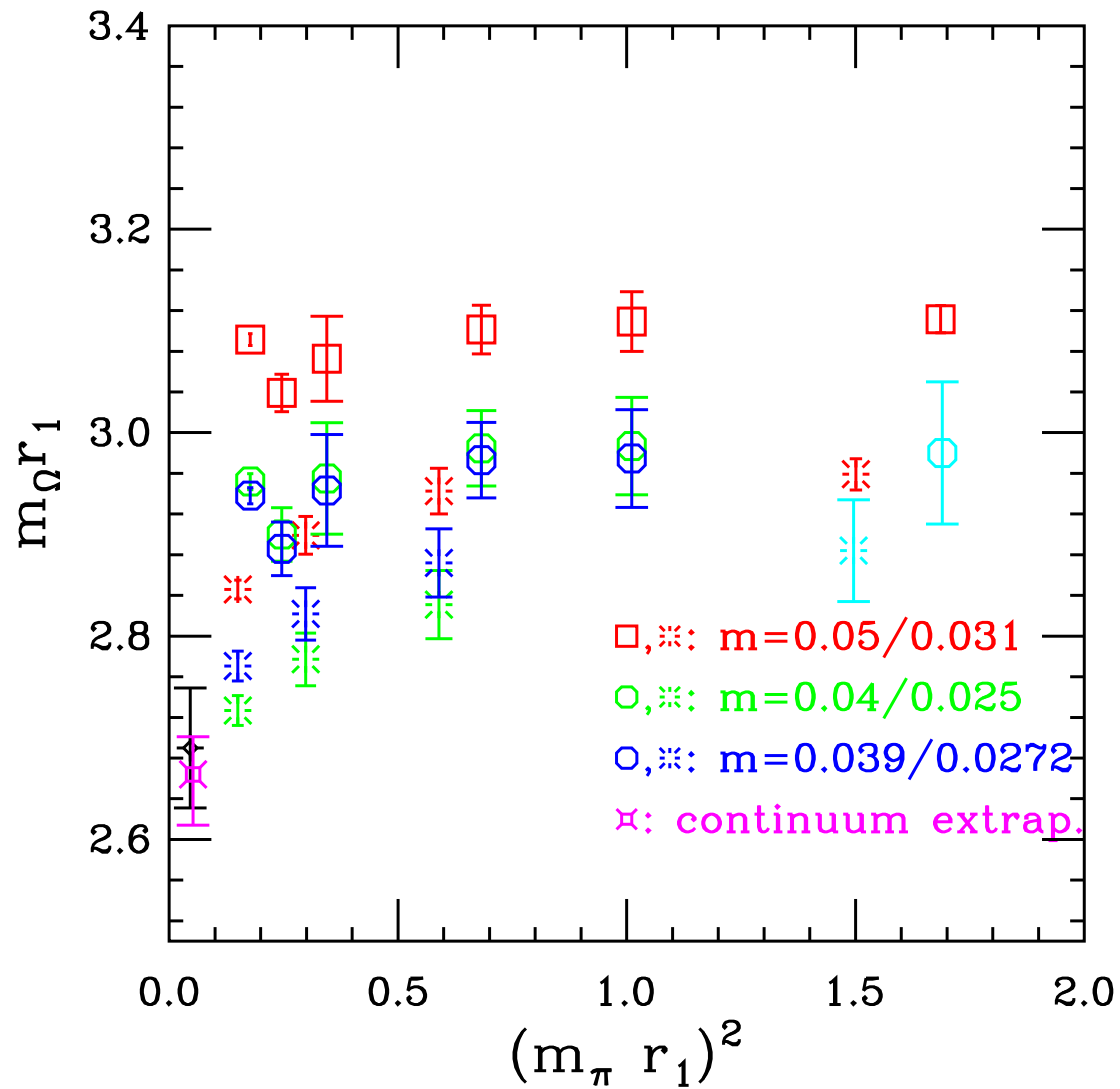
- Consistent with “conventional results” summarized, e.g., in Cohen, Kaplan, & Nelson, JHEP 9911, 027 (1999):  
 $L_5 = 2.2(5)$ ,  $L_6 = 0.0(3)$ ,  $L_4 = 0.0(5)$ .
- Our result for  $2L_8 - L_5$  is far from range that would allow  $m_u = 0$ ,  $-3.4 \leq 2L_8 - L_5 \leq -1.8$  (Kaplan & Manohar; Cohen, Kaplan & Nelson)
- Consistent with (but not independent of) direct determination of  $m_u$ .

# Nucleon masses



The fancy plusses are continuum extrapolations at fixed  $m_\pi r_1$ . The curves are different continuum chiral extrapolations (with  $m_\pi^3$  term [3 lowest points], additional analytic  $m_\pi^4$  term [all 4 points, red curves];  $m_\Delta - m_N$  included, see V. Bernard *et al.* PLB 622 (2005) 141 [hep-lat/0503022] [green curve]; power series in  $m_\pi^2$  and  $\log(m_\pi^2)$  [blue curve]).

# $\Omega^-$ baryon





# Electroweak interaction and the CKM matrix

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The charged electroweak current couples the fermions of the Standard Model to the  $W$ -bosons

$$\mathcal{L}_{CC} = -\frac{g_w}{\sqrt{2}} J_{CC}^\mu W_\mu^+ + h.c.$$

At low energy,  $E \ll m_W$ , this leads to an effective current-current (4-Fermi) interaction

$$\mathcal{L}_{eff} = -2\sqrt{2}G_F J_{CC}^\mu J_{CC,\mu}^\dagger$$

with

$$G_F = \frac{g_w^2}{4\sqrt{2}M_W^2} = 1.16639(1) \times 10^{-5} GeV^{-2}$$

the Fermi constant.

# Electroweak interaction and the CKM matrix

The charged weak current is given by

$$J_{CC}^\mu = (\bar{\nu}_e, \bar{\nu}_\mu, \bar{\nu}_\tau) \begin{pmatrix} e_L \\ \mu_L \\ \tau_L \end{pmatrix} + (\bar{u}_L, \bar{c}_L, \bar{t}_L) V_{CKM} \begin{pmatrix} d_L \\ s_L \\ b_L \end{pmatrix} .$$

The **Cabbibo-Kobayashi-Maskawa (CKM) matrix** shows that the quark families mix in the weak interactions:

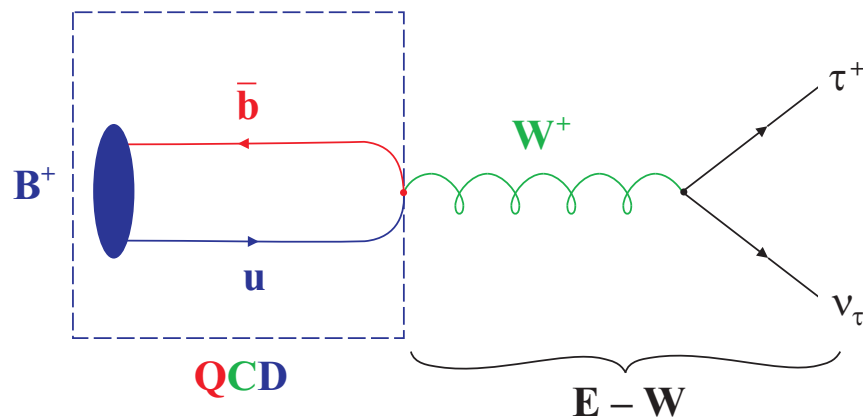
$$V_{CKM} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} .$$

The elements of the **CKM matrix** are parameters in the Standard Model that need to be **determined from experiment**. **Theoretical input, from lattice QCD, is needed for this.**

# Heavy-light decay constants

The leptonic decay branching ratio of a  $B$ -meson, and similarly a  $D$ -meson (or  $K^+$  or  $\pi^+$  mesons), goes like

$$B(B \rightarrow \ell \nu_\ell) = |V_{ub}|^2 f_B^2 m_\ell \left(1 - \frac{m_\ell^2}{m_B^2}\right) \times \text{known factors} .$$



So computing the **QCD** matrix element  $f_B$ ,

$$\langle 0 | \bar{b} \gamma_5 \gamma_\mu u | B(p) \rangle = i p_\mu f_B ,$$

is needed to extract the **CKM** matrix element  $V_{ub}$ .

# Heavy-light decay constants

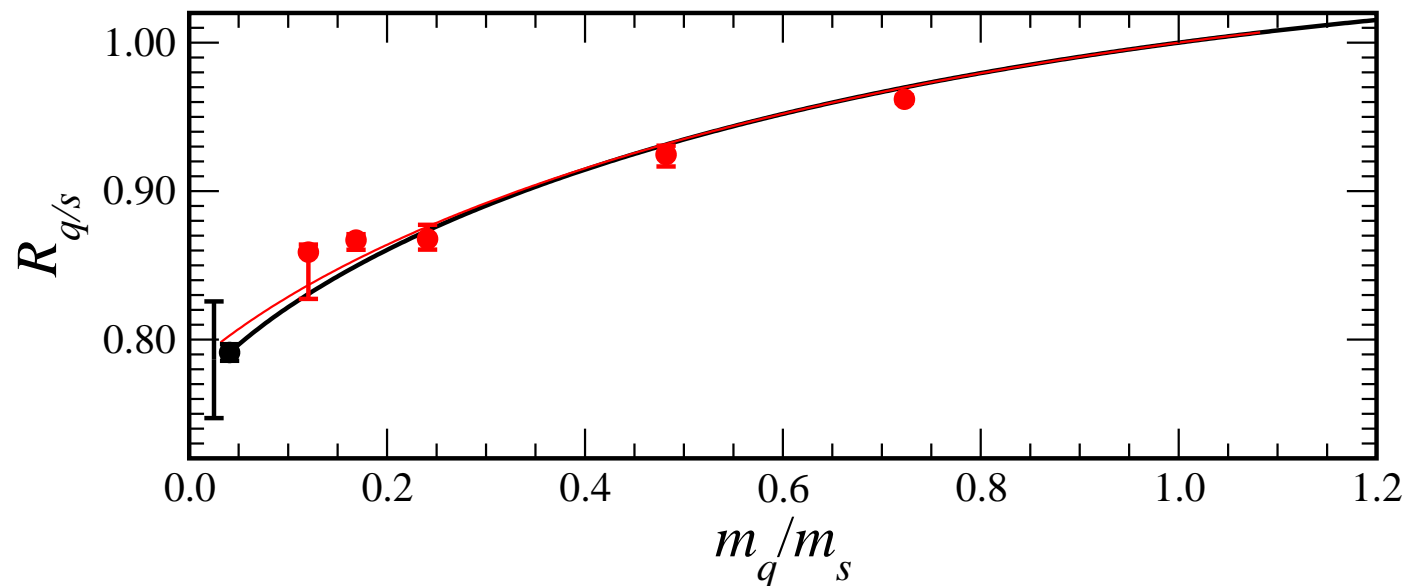
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With the Fermilab and HPQCD collaborations, we are computing the decay constant with improved staggered light and heavy clover (Fermilab) quarks. Advantages are:

- Can go to lower light valence quarks
- Use **SχPT** (Aubin & Bernard) for chiral extrapolation to  $m_d$
- Have  $Z$ -factors, written as  $Z_V^{Qq} = \rho_V (Z_V^{QQ} Z_V^{qq})^{1/2}$ , with  $Z_V^{QQ}$  and  $Z_V^{qq}$  from charge normalization, **non-perturbatively**, and  $\rho_V \approx 1$  **to one-loop**.

# Heavy-light decay constants

Use of **SχPT** is illustrated in the fit of  $R_{q/s} = f_D \sqrt{m_D} / f_{D_s} \sqrt{m_{D_s}}$ .  
The **red line and extrapolated point** are obtained after removing the  $\mathcal{O}(a^2)$  effects from the fit.



Details in C. Aubin *et al.*, PRL 95 (2005) 122002  
[hep-lat/0506030]

# Heavy-light decay constants

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We find:

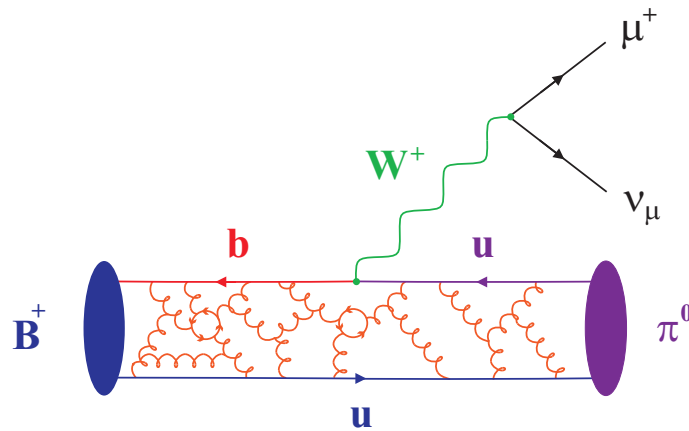
$$\begin{aligned}f_{D_s} &= 249 \pm 3 \pm 16 \text{ MeV} , \\f_D &= 201 \pm 3 \pm 17 \text{ MeV} , \\ \frac{f_{D_s} \sqrt{m_{D_s}}}{f_D \sqrt{m_D}} &= 1.27 \pm 0.06 \pm 0.06 .\end{aligned}$$

The computations for  $B$ -mesons are in progress.  
Experimentally measured, from leptonic decays

$$\begin{aligned}f_{D_s^+} &= 274 \pm 13 \pm 7 \text{ MeV} \quad (\text{CLEO}), \\f_{D_s^+} &= 283 \pm 17 \pm 7 \pm 14 \text{ MeV} \quad (\text{BABAR}), \\f_{D^+} &= 222.6 \pm 16.7_{-3.4}^{+2.8} \text{ MeV} \quad (\text{CLEO}), \\ \frac{f_{D_s^+}}{f_{D^+}} &= 1.23 \pm 0.11 \pm 0.04 .\end{aligned}$$

# Semileptonic B/D decays

With the Fermilab and HPQCD collaborations, we are computing also form factors for semileptonic  $D \rightarrow \pi/K$  and  $B \rightarrow \pi/D$  decays.



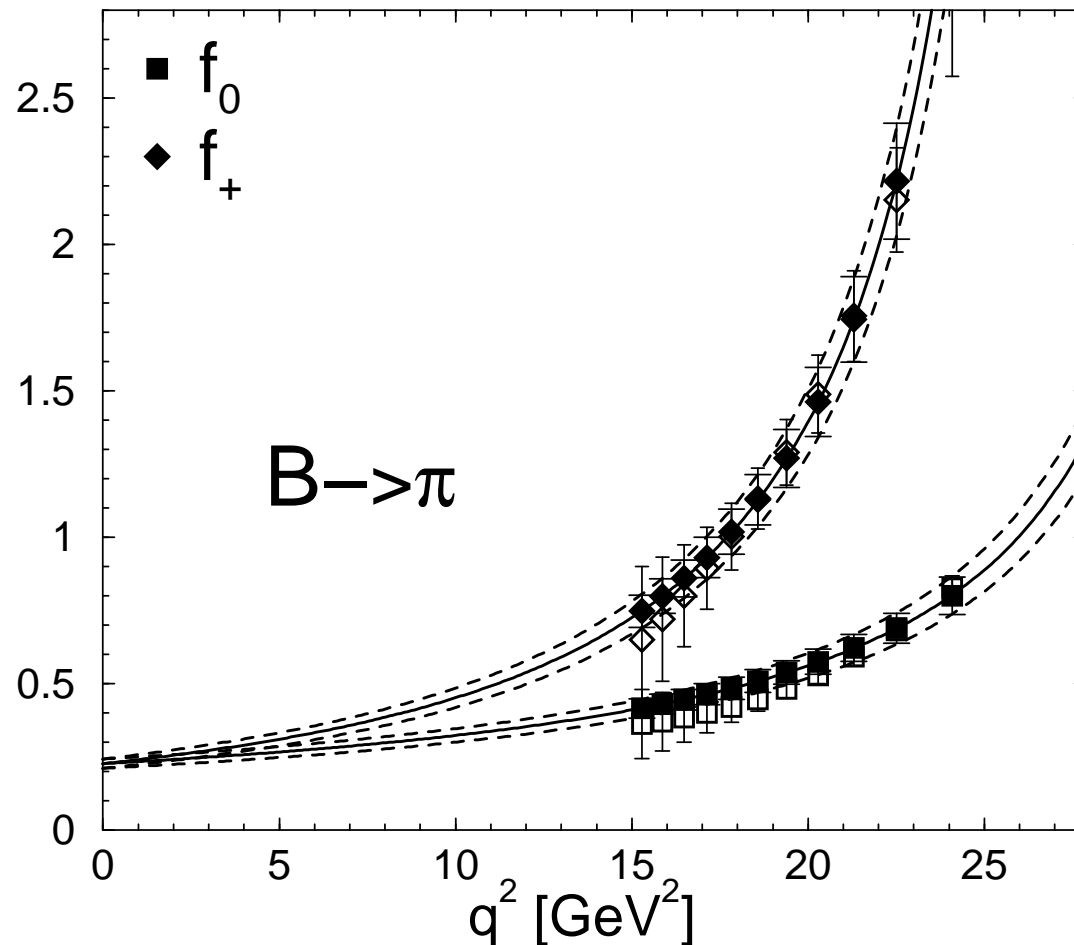
The heavy-to-light decay amplitudes, **non-perturbative QCD quantities**, are parametrized as

$$\langle P|V^\mu|H\rangle = f_+(q^2)(p_H + p_P - \Delta)^\mu + f_0(q^2)\Delta^\mu,$$

where  $\Delta^\mu = (m_H^2 - m_P^2)q^\mu/q^2$ .

# Semileptonic B/D decays

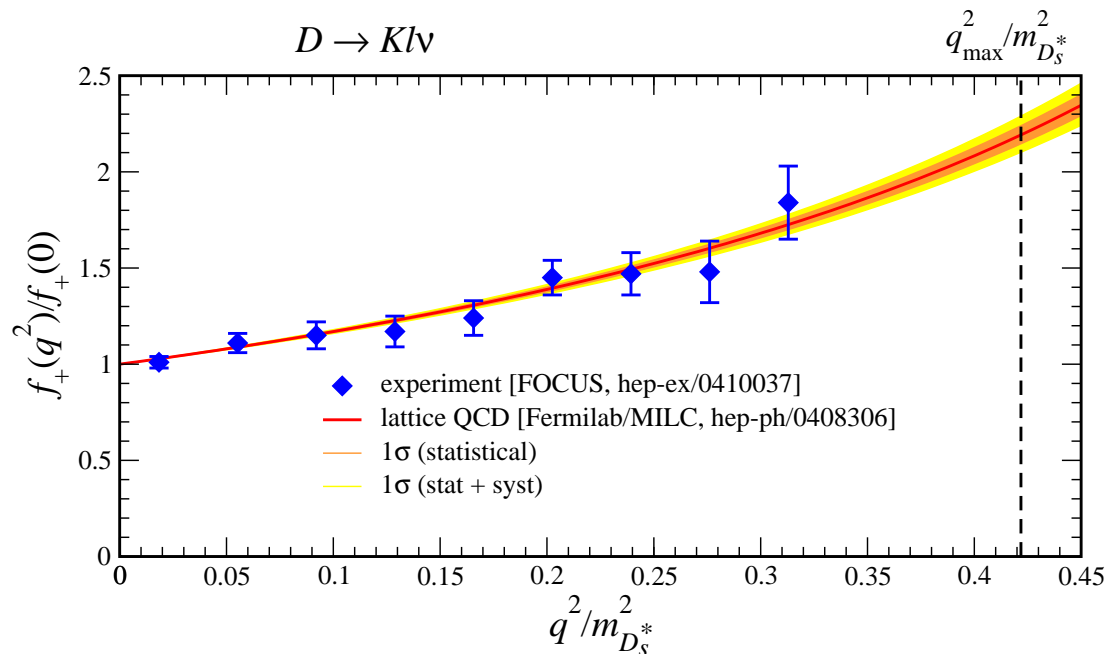
As an example we show the  $B \rightarrow \pi$  form factors  $f_0$  and  $f_+$ , see M. Okamoto *et al.*, hep-ph/0409116 (Lattice 2004):





# Semileptonic B/D decays

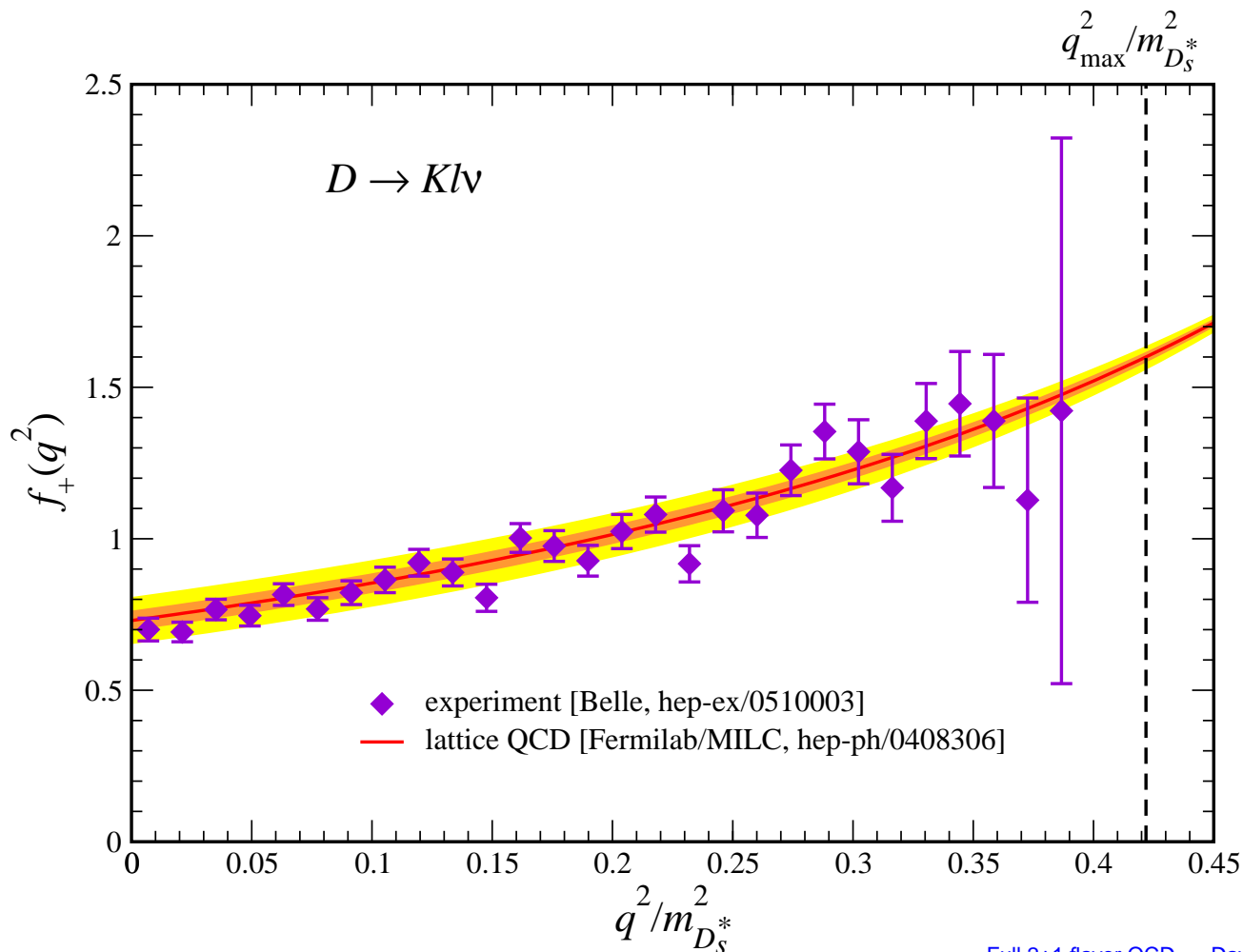
Our calculations has been compared to the experimental form factor  $f_+^{(K)}(q^2)$  for the process  $D^0 \rightarrow K^- \mu^+ \nu$  by the FOCUS collaboration (Phys. Lett. B607 (2005) 233 [hep-ex/0410037]).



see C. Aubin *et al.*, PRL 94 (2005) 011601 [hep-ph/0408306]

# Semileptonic B/D decays

Or, we can compare with the recent measurement by Belle, including the normalization (modulo assumptions on  $|V_{CS}|$ ):



# Semileptonic B/D decays

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The differential semileptonic decay rate is given by

$$\frac{d\Gamma}{dq^2} = \frac{G_F^2 p'^3}{24\pi^3} |V_{\text{CKM}}|^2 |f_+(q^2)|^2 .$$

$p'$ : 3-mom of final-state meson in restframe of initial-state meson.

Knowing  $f_+(q^2)$  allows us to extract CKM matrix elements from experiment. We find:

$$|V_{ub}| = 3.78(30)(42)(25) \times 10^{-3} , \quad |V_{cd}| = 0.239(10)(24)(20) ,$$

$$|V_{cs}| = 0.969(39)(94)(24) , \quad |V_{cb}| = 3.91(09)(34) \times 10^{-2} ,$$

with  $(|V_{cd}|^2 + |V_{cs}|^2 + |V_{cb}|^2)^{1/2} = 1.00(10) .$

# Summary and Outlook

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Simulations at two (and, in progress, more) lattice spacings and several sea quark masses in full 2+1 flavor QCD lead to **precision results in the pseudoscalar sector**, including decay constants,  $V_{us}$  and quark masses.

Many other “gold-plated” observables also show good agreement with experiment.

The configurations are used for predictions for heavy-light meson decay constants and semileptonic form factors, needed for extraction of CKM matrix elements from experiments.

Improvements will include:

- Simulations with a smaller strange sea quark mass (done for  $a = 0.12$  fm, planned for  $a = 0.09$  fm)
- Full analysis of coarser ensembles, 0.18 and 0.15 fm
- More light quark masses, and more statistics, for the smaller lattice spacing:  $a \sim 0.06$  fm

# Spectrum summary

