The Future of Lattice Calculations

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Outline

- Brief discussion of systematics on lattice
- Issues with staggered fermions
- What quantities can be calculated well on the lattice?
- State of the art (focus on f_π, f_K — model for heavy-light calculations we want to do)
- One more important systematic error
- What precision can be expected, and when?

Systematic Errors

Chiral extrapolation:

- Computer time rises like large power of $1/m_{u,d}$ as these masses approach their physical values.
- Must work with larger masses and extrapolate; use chiral perturbation theory (χPT) to guide extrapolation.
  - "Partially quenched" χPT ($m_{\rm val} \neq m_{\rm sea}$) esp. useful.
  - Note: as long as there are 3 flavors of sea quarks, partially quenched world has real world as a subset.
- Essentially all interesting quantities with light (u, d) quarks have significant curvature $\sim m_\pi^2 \ln(m_\pi^2/\Lambda_\chi^2) \Rightarrow$ must get to small quark mass (probably $m_{u,d} \sim m_s/4$ to $m_s/8$) to control chiral logs in extrapolation.
- If only have large mass ($m_{u,d} \gtrsim m_s/2$), will be stuck with 10% or even 20% errors (Kronfeld & Ryan).

Systematic Errors

Quenching:

- Most lattice calculations to date have left out the effects of sea quarks.
- Reduces computer time by large factor: $\sim$100–1000 or more.
- But an uncontrolled approx: errors 10%–20% or more.
- Need to move beyond quenching for lattice to fulfill promise & have an impact on phenomenology.
- Dynamical (sea quark) masses must be small: otherwise just trading quenching error for chiral extrap error.
- In near term only "staggered" quarks are viable:
  - very fast
  - have residual chiral symmetry that protects from "exceptional configurations" $\Rightarrow$ can go to low quark mass

Systematic Errors

Discretization Effects (finite lattice spacing a):

- Order of errors in a depends on fermion action:
  - Wilson: $\mathcal{O}(a)$
  - Improved Wilson ("clover") (perturbative): $\alpha_S^2 \mathcal{O}(a)$
  - Improved Wilson ("clover") (nonperturbative): $\mathcal{O}(a^2)$
  - Staggered: $\mathcal{O}(a^2)$
  - Improved staggered ('Asqtad"): $\mathcal{O}(\alpha_S a^2)$
  - Domain wall: $\mathcal{O}(a^2)$
  - Overlap: $\mathcal{O}(a^2)$
- Now & foreseeable future: if few % accuracy is desired, discretization errors are not negligible at fixed a for any action.
- Must extrapolate to continuum ($a \to 0$) using known leading a dependence.

Systematic Errors

Finite Volume:

- Depends on how many hadrons are in initial or final state:
  - More than 1 hadron $\Rightarrow$ probably out of reach in next five years for all but the most qualitative studies.
  - Single particles $\Rightarrow$ currently feasible volumes are enough to reduce finite volume effects to few % level (without major sacrifice on discretization errrors).
  - Typically $V \gtrsim (2.5\mathrm{fm})^2$ will do the job.

Systematic Errors

Finite Volume:

- Can do even better for single-particle quantities whose mass dependence is determined by χPT.
- χPT predicts the volume dependence (for large volume), so can correct for finite volume effects $\Rightarrow$ negligible errors ($\sim 0.1\%$).
- Ignore finite volume effects for single-particle states from here on.

Systematic Errors

"Setting the Scale"

- Lattice spacing a is determined after the fact by comparing the result for one dimensional quantity with experiment. (Equivalent to fixing Λ_{QCD} or α_S.)
- So lattice error in the quantity used to set the scale will infect all other dimensionful results.
- The best we can do today is probably from Υ splittings: 2S-1S or 1P-1S: gives about 2% scale error.
- The scale error is usually negligible on dimensionless ratios (like f_{B_s}/f_B), but is not strictly 0. (Error can enter indirectly through determination of quark masses or momenta.)

Staggered Baggage

Staggered quarks have an incomplete reduction of lattice doubling symmetry

- Each staggered lattice field (each staggered flavor) $\Rightarrow$ 4 equivalent particles in continuum.
- The quantum number of this unphyical multiplication of d.o.f. is called “taste.”
- Taste symmetry, while presumably exact in the continuum, is violated on the lattice at $\mathcal{O}(\alpha^2 a^2)$ (for improved staggered).
- Although formally non-leading (leading discretization errors are $\mathcal{O}(\alpha a^2)$), taste violations are numerically important.
- Leads to both practical and theoretical issues.

Staggered Baggage

- Practical issue: taste violations must be taken into account in χPT used for extrapolation in light quark mass.
  - Need to fit finite-a lattice data to "staggered chiral perturbation theory" (SχPT).
  - SχPT has been worked out (Lee & Sharpe; Aubin & C.B.) for π-K system.
  - Applying SχPT to heavy-light mesons should be straightforward, but has not yet been done.
  - Will present future error estimates with & without assumption that heavy-light SχPT will have been worked out.

Staggered Baggage

- Theoretical issue: need to eliminate taste degree of freedom for quarks in simulations (need 1 flavor – 1 quark).
  - For valence quarks, taste is simply an annoyance: just choose external quarks to have a single taste.
  - But for dynamical quarks, must reduce tastes to 1 per flavor by taking $\sqrt[4]{\mathrm{Det}}$
  - At finite lattice spacing this is nonlocal operation. Could it introduce nonuniversal behavior; nonlocality in the continuum?
    - $\sqrt[4]{\mathrm{Det}}$ is correct at every finite order of perturbation theory.
    - Also some significant nonperturbative evidence against this disaster (and no evidence for it), but many reasonable people remain unconvinced.

Staggered Baggage

- Estimates below on what can be done on lattice assume that staggered quarks are ok: give QCD in the continuum limit.
- If not, safer but slower methods can be used, but they will lead to much larger systematic errors for the quantities you want to know.

Gold-plated Quantities

So what quantities can the lattice compute well (few %) in the next ~ 5 years?

- At most one hadron in initial and final state
  - large enough volume, small enough a are then feasible for unquenched theory.
- Stable hadrons, not near thresholds
  - No ρ or K^*, sorry!
  - Unstable particles require very large volumes (and untested techniques) to treat decay products correctly
  - Decays like $B \to \rho$ will be calculated, but errors will not be very well controlled ($\sim 10\%$?) — model dependence in answers and error estimates.
  - $B \to D^* \ell \nu$ may be an exception because model dependence multiplies $\mathcal{F}(1) - 1$.

Gold-plated Quantities

So what quantities can the lattice compute well (few %) in the next ~ 5 years?

- The η also probably excluded. [Need to include η-η' mixing $\Rightarrow$ disconnected graphs $\Rightarrow$ difficult]
- No high momenta (need $|\vec{p}|a \ll 1$).
  - probably limited to $|\vec{p}| \lesssim 1\mathrm{GeV}$
  - $\Rightarrow q^2 \gtrsim (17\ \mathrm{GeV})^2$ for $B \rightarrow \pi$ semileptonic form factors.
  - prob. also need $q < q_{\mathrm{max}}$ to avoid B^* pole at end point. (Minimum lattice momentum for fixed lattice size may then require $|\vec{p}| \gtrsim 350\ \mathrm{MeV}$ or more.)
- Chiral extrapolation must be under good control
- We call such quantities "gold-plated" = "no excuses"

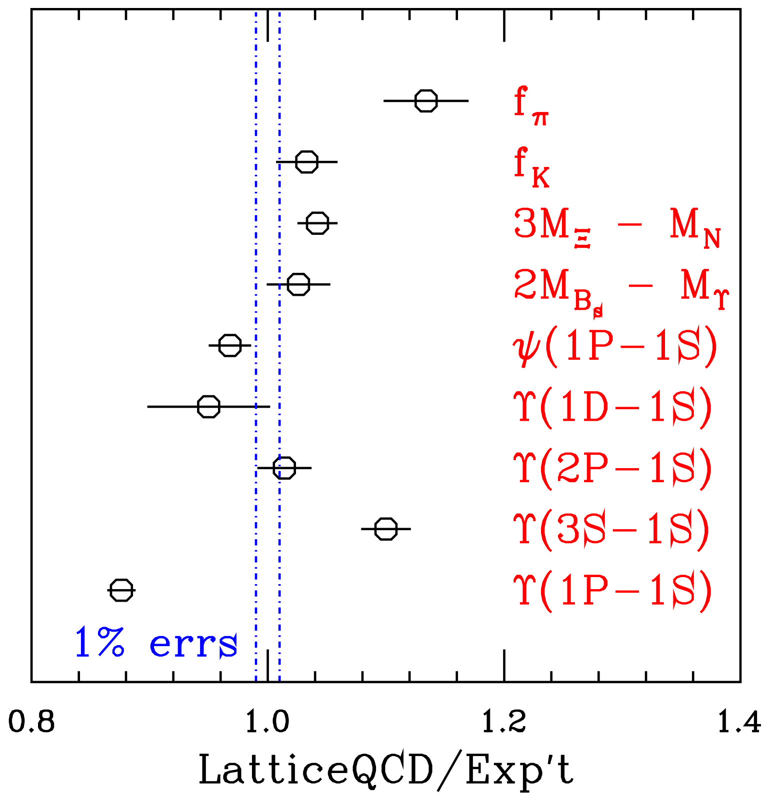
State of the Art

MILC configurations

- Since 1999, MILC collaboration has been generating lattice configurations including three sea-quark flavors (u, d, s), using improved staggered quarks (with $m_u = m_d$).
- Large sample at $a \approx 0.125$ fm and $L \approx 2.5$ fm.
  - Wide range of sea quark masses
  - Lowest $m_{u,d} \sim 10$ MeV (“m_π” $\approx 260\ MeV$).
- Smaller sample at $a \approx 0.09$ fm, $L \approx 2.5$ fm still being generated.
  - Two low-mass sets completed
  - Lowest $m_{u,d} \sim 15$ MeV (“m_π” $\approx 320\ MeV$).
  - Working on $m_{u,d} \sim 10$ MeV (“m_π” $\approx 260\ MeV$).
- Configurations publicly available:
  `http://qcd.nersc.gov/`

State of the Art

Results with existing MILC configurations ("MILC0 set")
(C. Davies, *et al.*, hep-lat/0304004)



Quenched Approximation

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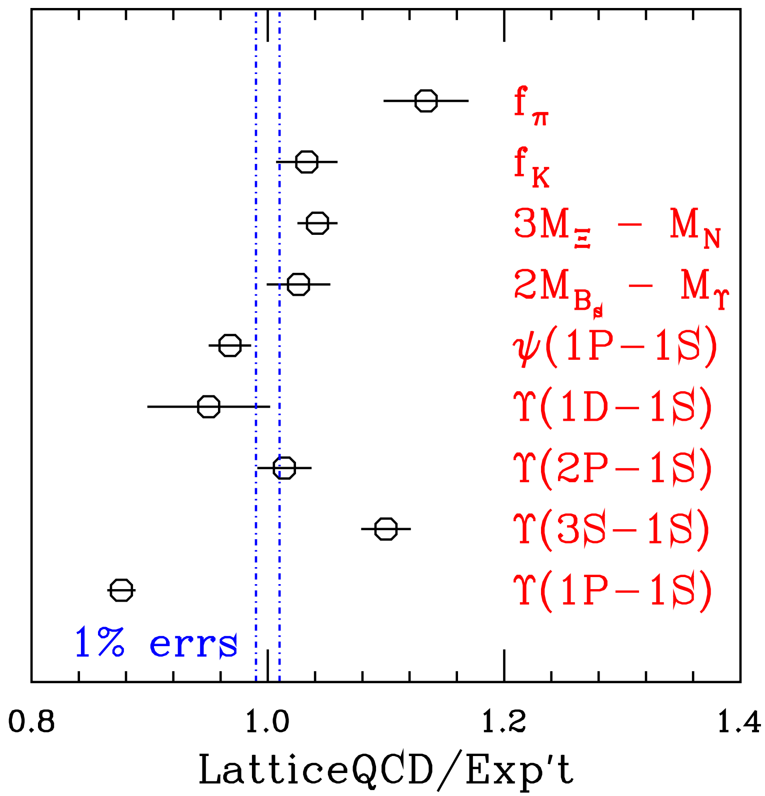
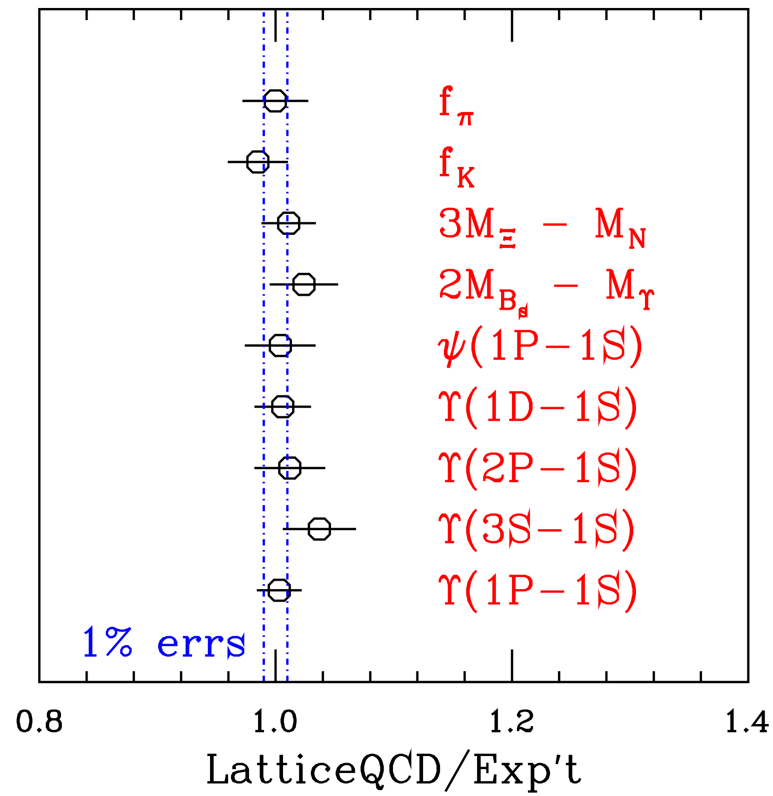


Quenched Approximation



Full QCD ($n_F = 3$)

[scale from Υ 2S-1S; $m_{u,d}, m_s, m_c, m_b$ from $m_\pi, m_K, m_{D_s}, m_\Upsilon$]

π-K System

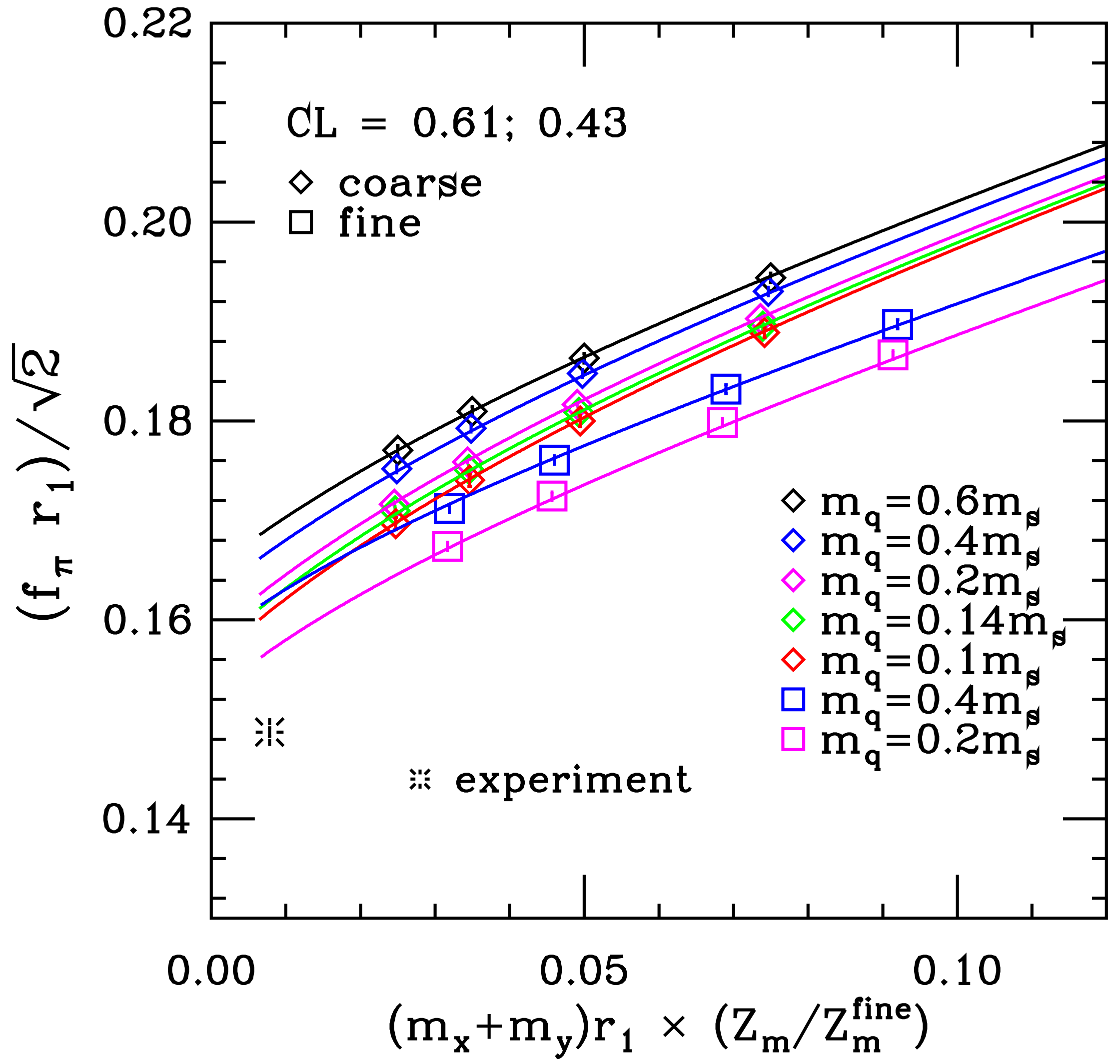
Current MILC calculation of f_π and f_K

- Closest existing example to future calculations of heavy-light leptonic and semileptonic decay constants.
- Basis of the error estimates to follow.

π-K System

Current MILC calculation of f_π and f_K

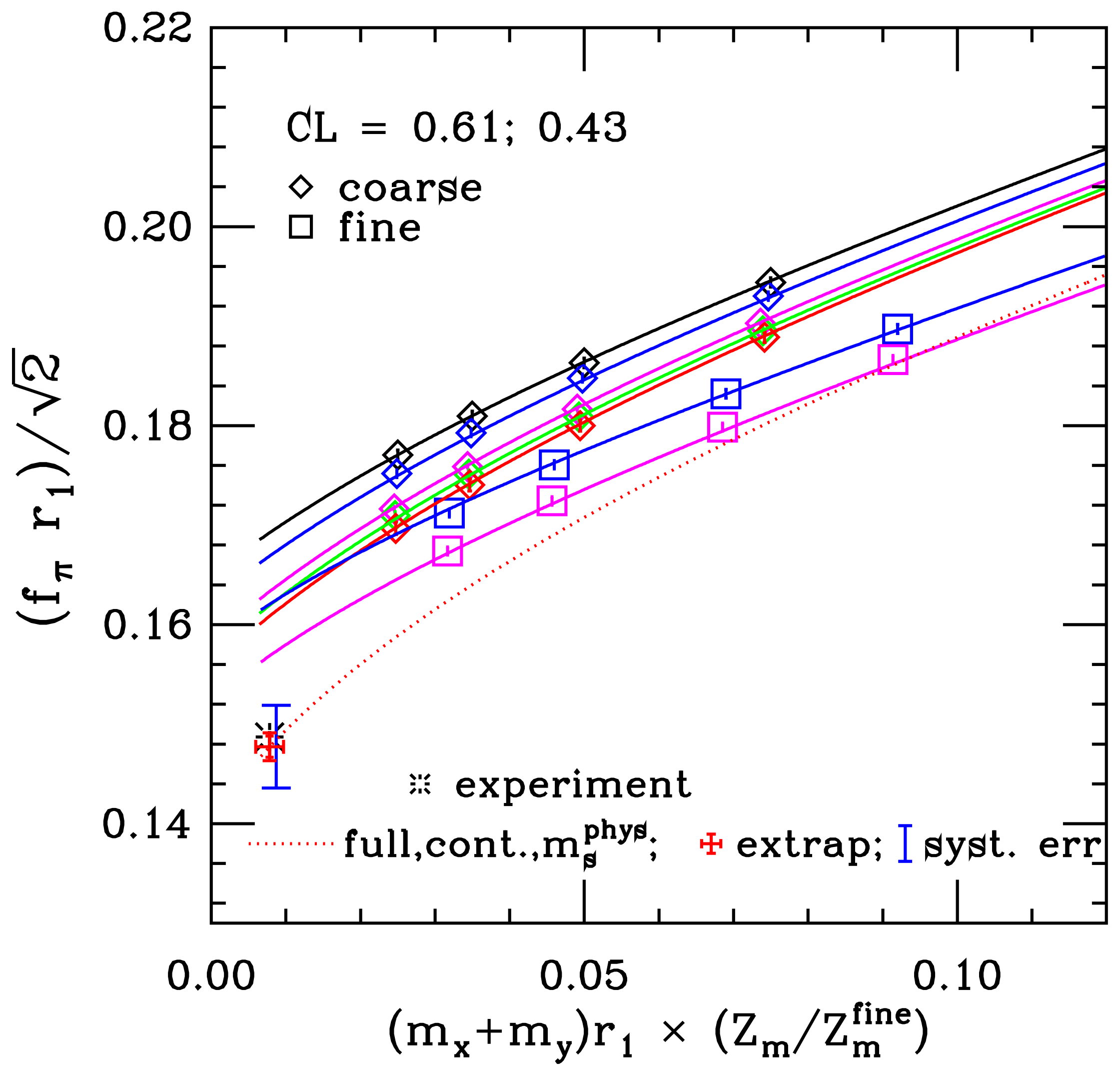
- Fit partially quenched data to PQχPT.



π-K System

Current MILC calculation of f_π and f_K

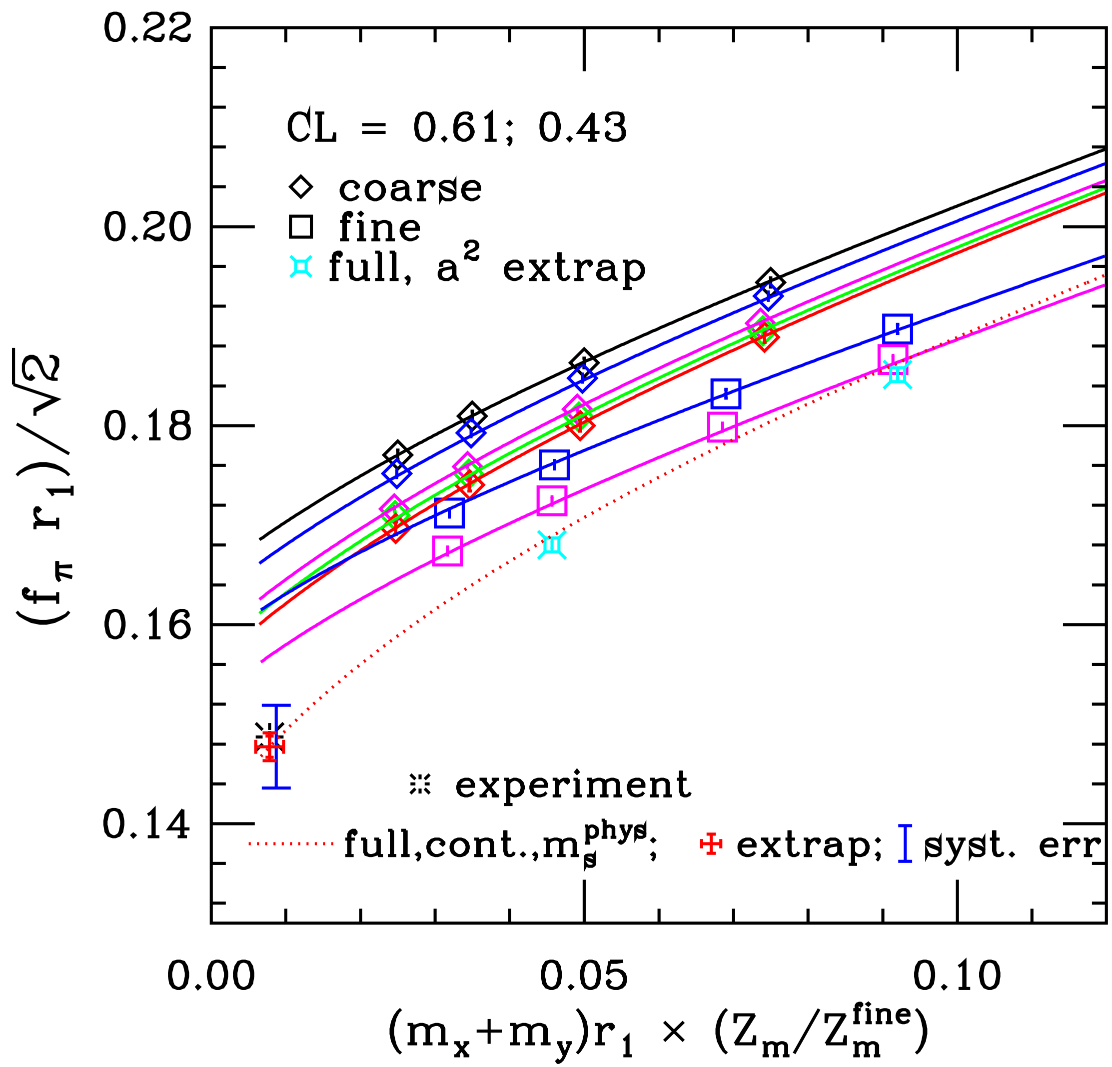
- Extrapolate fit params to continuum
- Set $m_{sea} = m_{val}$ and plot a function of m_{val} (⋯⋯⋯)
- Set $m_{val} = m_{u,d}^{\rm phys}$ (determined from m_π).



π-K System

Current MILC calculation of f_π and f_K

- Consistency check: extrapolate points with $m_{val} = m_{sea}$ to continuum at fixed quark mass.



Systematic Errors (*cont. . .*)

Perturbation theory:

- For f_π, f_K, we are lucky: staggered lattice PCAC $\Rightarrow$ light-light axial current not renormalized $\Rightarrow$ lattice & continuum currents are the same.
- But many interesting gold-plated quantities (*e.g.*, heavy-light leptonic & semileptonic decay constants) require perturbative calculation (or equivalent nonperturbative lattice computation) to match lattice current to continuum current.
- In new era of unquenched, light mass simulations, one-loop calculations have unacceptably large errors ($\sim$10%).
- But lattice perturbation theory very messy (complicated actions; no Lorentz invariance).

Systematic Errors (*cont. . .*)

Perturbation theory:

- Probably need "automated perturbation theory," (Trottier, Lepage, & collabs.), based on work by Lüscher & Weisz.
  - My reading: no difficulties in principle with going to 2 or even 3 loops.
  - However, still some practical problems that need to be overcome:
    - Issues of IR regulation important
    - currently use "twisted boundary conditions" on lattice
    - to match to continuum, need to use same twisted boundary conditions there.
    - continuum perturbation theory (dim reg?) with twisted b.c. hard

Systematic Errors (*cont. . .*)

Perturbation theory:

- Will present future error estimates with & without assumption that 2-loop perturbative matching will exist.
- Luckily, many interesting quantities, *e.g.*, ratios like f_{B_s}/f_B, are independent or nearly independent of perturbation theory.

Future Lattice Precision

- Fermilab/MILC collaboration now beginning computations of heavy-light semi-leptonic form factors and leptonic decay constants:
  - Dynamical (sea quark) configurations are the existing improved staggered $n_F = 3$ MILC ones ("MILC0").
  - Valence light quarks will also be staggered, so chiral regime reachable.
  - CPU requirements are relatively small since dynamical configurations already exist.
  - With time for analysis, I estimate this calculation can be completed in 1-2 years.
  - Estimates for future precision will be much more reliable once this $0^{\rm th}$ generation project is completed.

Future Lattice Precision

- Next steps will require new dynamical configurations (lighter quark mass, smaller lattice spacing):
  - MILC1
    - ~ 6 Teraflop-years
    - Machines now being built: Columbia QCDOC; large clusters (SciDAC project)
    - ETA: 3-5 years (including analysis time)
  - MILC2
    - ~ 50-100 Teraflop-years
    - Next generation of machines
    - ETA: 5-8 years (including analysis time)

Future Lattice Precision

- Next steps will require new dynamical configurations (lighter quark mass, smaller lattice spacing):
  - DWF1: Dynamical domain wall fermions (or equivalent) at comparable mass and spacings to MILC1
    - Comparable precision to MILC2 because no taste violations
    - Safe from all staggered baggage
    - ~ 1000 Teraflop-years
    - “Next next” generation of machines
    - ETA: 10 years (including analysis time)

Future Lattice Precision

- Error estimates to follow are based on DOE planning document prepared by S. Sharpe, C.B., A. El-Khadra, P. Mackenzie, and R. Sugar.
- However, I have tweaked those estimates using my own expectations/prejudices.

MILC0 error estimates

quantity	statist.	scale	light q		heavy Q	pert. th.	
			no SχPT	SχPT		1-loop	2-loop
f_B	3	2	5	2.5	3	7.5	2
$f_B\sqrt{B_B}$	4	2	5.5	3	3	8.5	2.5
f_{B_s}/f_B	1	–	5	2.5	1	–	–
ξ	2	–	5.5	3	1	–	–
$B \to \pi\ell\nu$	4.5	1	6	3	3	7.5	2
$B \to D\ell\nu$	1	0.5	2	1	1	2.5	0.7

Estimated per cent errors. "Light q" includes light quark chiral and discretization errors. "Heavy Q" means heavy quark discretization errors. Semileptonic form factors are for restricted range $0.5\ \text{GeV} \lesssim \vec{p}_\pi \lesssim 1\ \text{GeV}$ (in B rest frame), but can have any bilinear current. $B \to D^*\ell\nu$ may be comparable to $B \to D\ell\nu$.

MILC1 error estimates

quantity	statist.	scale	light q		heavy Q	pert. th.	
			no SχPT	SχPT		1-loop	2-loop
f_B	2	1.5	3	1.5	2	7.5	2
$f_B\sqrt{B_B}$	3	2	3.5	2	2	8.5	2.5
f_{B_s}/f_B	0.8	–	3	1.5	0.8	–	–
ξ	2	–	3.5	2	1	–	–
$B \to \pi\ell\nu$	3	0.7	4	2	2	7.5	2
$B \to D\ell\nu$	0.6	0.5	2	1	0.6	2.5	0.7

Estimated per cent errors. "Light q" includes light quark chiral and discretization errors. "Heavy Q" means heavy quark discretization errors. Semileptonic form factors are for restricted range $0.35\ \mathrm{GeV} \lesssim \vec{p}_\pi \lesssim 1\ \mathrm{GeV}$ (in B rest frame), but can have any bilinear current. $B \to D^*\ell\nu$ may be comparable to $B \to D\ell\nu$.

MILC2 error estimates

quantity	statist.	scale	light q		heavy Q	pert. th.	
			no SχPT	SχPT		1-loop	2-loop
f_B	1	1	2	1	1.5	7.5	2
$f_B\sqrt{B_B}$	1.3	2	2.5	1	1.6	8.5	2.5
f_{B_s}/f_B	0.5	–	2.5	1	0.5	–	–
ξ	1	–	3	1	0.6	–	–
$B \to \pi\ell\nu$	1.5	0.5	2.7	1.3	1.5	7.5	2
$B \to D\ell\nu$	0.3	0.3	1.4	0.7	0.5	2.5	0.7

Estimated per cent errors. “Light q” includes light quark chiral and discretization errors. “Heavy Q” means heavy quark discretization errors. Semileptonic form factors are for restricted range $0.35\ \mathrm{GeV} \lesssim \vec{p}_\pi \lesssim 1\ \mathrm{GeV}$ (in B rest frame), but can have any bilinear current. $B \to D^*\ell\nu$ may be comparable to $B \to D\ell\nu$.

Summary error estimates (%)

quantity	now	1-2 yrs. MILC0	3-5 yrs. MILC1	5-8 yrs. MILC2
f_B	15	10, 9, 7, 6	9, 8, 5, 4	8, 8, 4, 3
$f_B\sqrt{B_B}$	15-20	12, 11, 8, 7	10, 10, 6, 5	9, 9, 5, 4
f_{B_s}/f_B	6	5, 3	3, 2	3, 1
ξ	7	6, 4	4, 3	3, 1.5
$B \to \pi\ell\nu$	15	11, 10, 8, 7	9, 9, 6, 5	8, 8, 4, 3
$B \to D\ell\nu$	6	4, 3, 3, 2	3, 3, 2, 1.6	3, 3, 2, 1.2

Key: red= NO SχPT; 1-loop pert. th.
purple= SχPT; 1-loop pert. th.
navy= NO SχPT; 2-loop pert. th. (or pert. th. not needed)
blue= SχPT; 2-loop pert. th. (or pert. th. not needed)

Summary error estimates (%)

quantity	now	1-2 yrs. MILC0	3-5 yrs. MILC1	5-8 yrs. MILC2
f_B	15	10, 9, 7, 6	9, 8, 5, 4	8, 8, 4, 3
$f_B\sqrt{B_B}$	15-20	12, 11, 8, 7	10, 10, 6, 5	9, 9, 5, 4
f_{B_s}/f_B	6	5, 3	3, 2	3, 1
ξ	7	6, 4	4, 3	3, 1.5
$B \to \pi\ell\nu$	15	11, 10, 8, 7	9, 9, 6, 5	8, 8, 4, 3
$B \to D\ell\nu$	6	4, 3, 3, 2	3, 3, 2, 1.6	3, 3, 2, 1.2

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blue= SχPT; 2-loop pert. th. (or pert. th. not needed)

= my best guess of what will be available

Hope for the future

- 5 or more years from now, it may become feasible to do "no-excuses" calculations on unstable particles
- $B \to \rho\ell\nu$, $B \to K^*\gamma$ may have errors comparable to $B \to \pi\ell\nu$ on MILC0

Disclaimers

- Errors on predicted errors are at least 30% (and that's "1σ").
- Errors on predicted errors increase as we move further into the future.