STATUS OF LATTICE QCD:

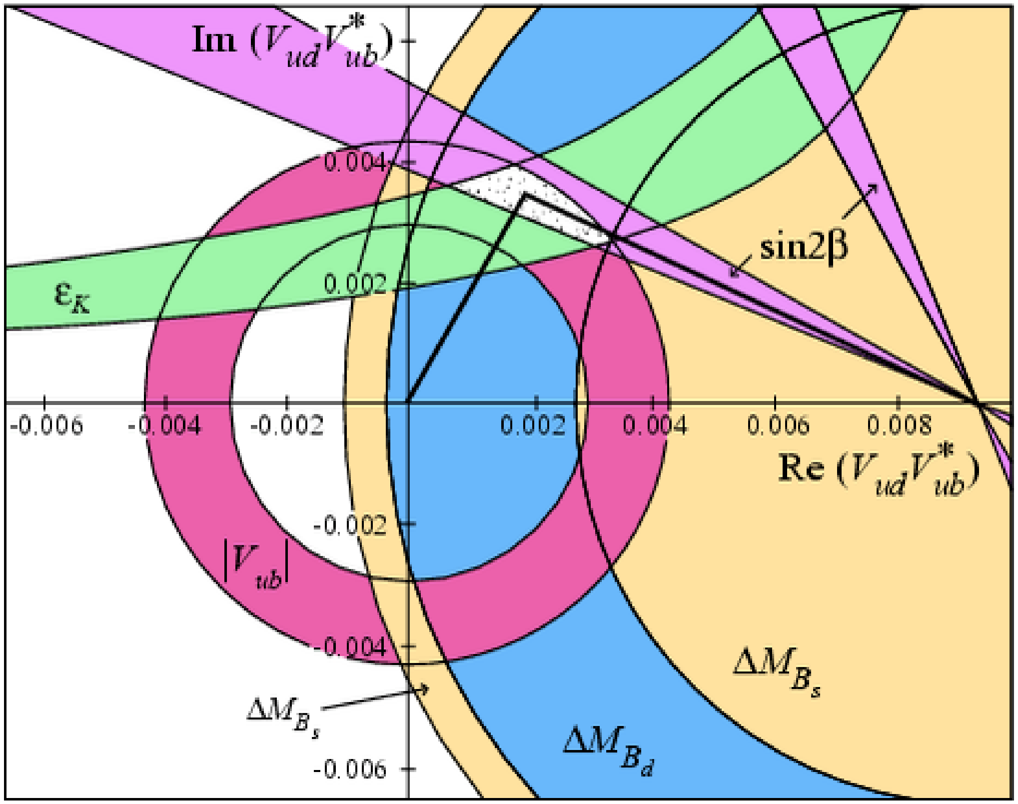
Implications for Flavor Physics

Andreas S. Kronfeld

Fermilab

8 October 2003

Unitarity Triangle



$$V_{ud}V^*_{ub} + V_{cd}V^*_{cb} + V_{td}V^*_{tb} = 0$$

PDG 2003

theoretical uncertainties dominate

Hadronic Matrix Elements

$$d\Gamma(B \to D^* l\nu) \propto |V_{cb}|^2 \mathcal{F}(1)^2 \qquad \langle D, v, \varepsilon | \varepsilon \cdot A | B, v \rangle = 2\sqrt{m_{D^*} m_B}\, \mathcal{F}(1)$$

$$d^2\Gamma(B \to \pi l\nu) \propto |V_{ub}|^2 f_+^2 \qquad \langle \pi | V^\mu | B \rangle = \sqrt{2m_B}\left[v^\mu f_\parallel + p_\perp^\mu f_\perp \right]$$

$$\sqrt{2m_B} f_+ = (m_B - E_\pi) f_\perp + f_\parallel$$

$$\Gamma(B \to l\nu) \propto |V_{ub}|^2 f_B^2 \qquad \langle 0 | A^\mu | B \rangle = m_B v^\mu f_B$$

$$\Delta m_q \propto |V_{tq}|^2 \eta_B \tfrac{8}{3} m_{B_q}^2 f_{B_q}^2 B_{B_q} \qquad \langle \bar{B}_q^0 | Q^{\Delta B=2} | B_q^0 \rangle = \tfrac{8}{3} m_{B_q}^2 f_{B_q}^2 B_{B_q}$$

Each hadronic matrix element is a well-defined property of hadrons.

Relatively simple: at most one hadron appears in the initial or final state.

Similar matrix elements enter in other places in flavor physics:
K^0-$\bar{K}^0$ mixing, $B \to K^*\gamma$, $B \to K^* l^+ l^-$, $D_{(s)}$ (semi-)leptonic decays, $\Delta\Gamma$.

A Dream?

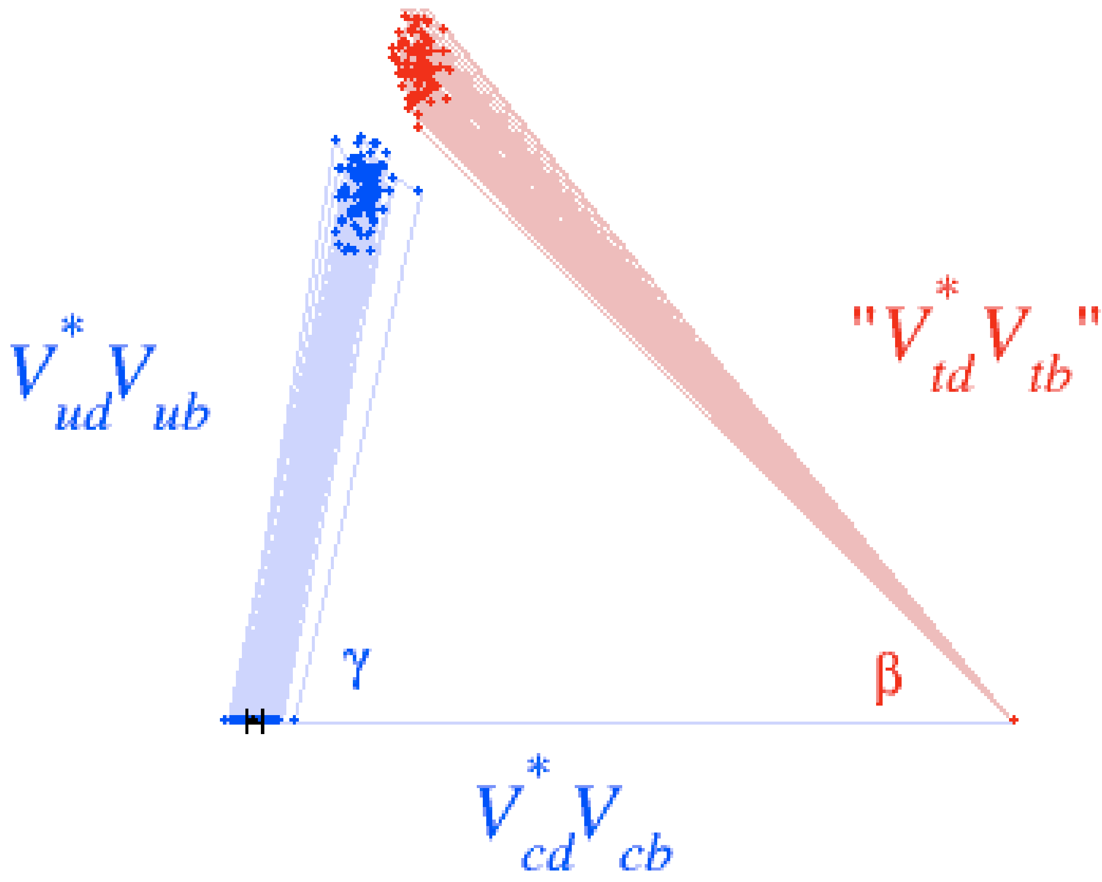
Suppose the theory could improve so that the errors are

$$\begin{array}{rcl} \mathcal{F}(1) \text{ – hence } & |V_{cb}| : & 1\% \\ f_+(1\text{ GeV}) \text{ – hence } & |V_{ub}| : & 4.5\% \\ B \to KD \text{ – hence } & \gamma : & 3\% \end{array}$$

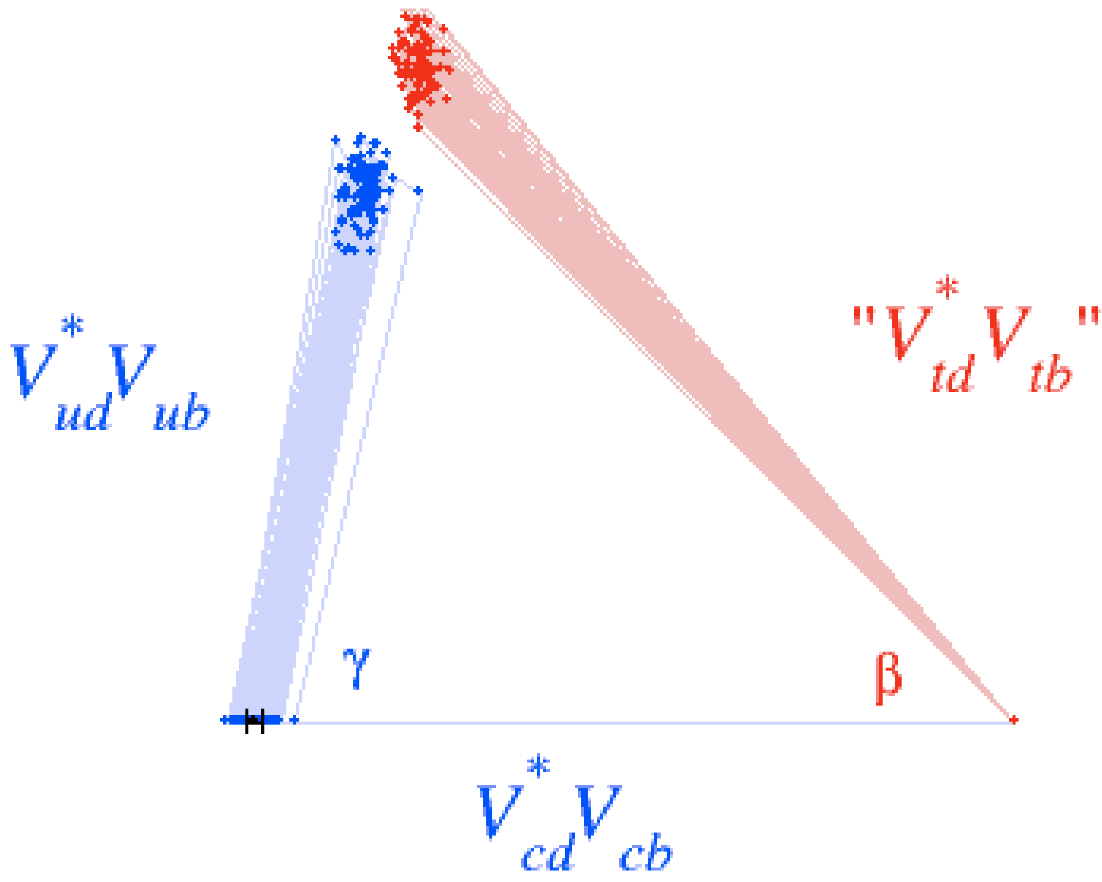
$$\begin{array}{rcl} f_B\sqrt{B_B} \text{ – hence } & \text{“}|V_{td}|\text{”}: & 4.5\% \\ B \to \psi K_S \text{ – hence } & \text{“}\beta\text{”} : & 2.5\% \end{array}$$

First three would determine $(\bar{\rho}, \bar{\eta})$ with tree topologies only.

Second two would test whether B^0-$\bar{B}^0$ mixing arises solely from the Standard box diagrams.


$V^*_{ud}V_{ub}$
"$V^*_{td}V_{tb}$"
γ
β
$V^*_{cd}V_{cb}$

The Matrix Reloaded



Quenched Lattice QCD

To reduce the computational burden, until now almost all numerical calculations of physically interesting masses or hadronic matrix elements have been done in the so-called "quenched approximation."

The quenched approximation omits vacuum quark loops, and compensates the omission by changing the bare gauge coupling and masses *ad hoc*.

Reminiscent of a dielectric approximation, $g_0^2 \to g_0^2/\varepsilon$, $m_{0q} \to m_{0q}/\rho$.

In practice: different adjustments of the $1+n_f$ bare parameters were needed for light, heavy-light, and heavy-heavy hadrons.

In the dielectric analogy, $\varepsilon(\omega)$, $\rho(\omega) \neq \text{constant}$.

Bottom line: quenching leaves unquantifiable uncertainties of 5–30%.

$2+1$ Flavors

Over the last few years, the MILC Collaboration has generated $10+4$ unquenched ensembles of lattice gauge fields.

$n_f = 3$ or $2+1$ flavors of quark loops: light $m_u = m_d \equiv m_l$ & strange m_s.

Ensemble: choice of $g_0^2(a)$, m_l^{sea}, m_s^{sea}; compute functional integrals numerically.

Light quark masses: $0.15 < m_l/m_s < 1$ the lightest available.

Improved staggered quarks with the Asqtad action: discretization errors of $O(\alpha_s a^2)$ and $O(a^4)$; $a = \frac{1}{8}$, $\frac{1}{11}$ fm. $L = 2.5$ fm.

Typically 500–600 configurations in each ensemble $\Rightarrow$
raw simulation data have statistical uncertainty $<$ few %.

MILC made the ensembles of gauge fields freely available.

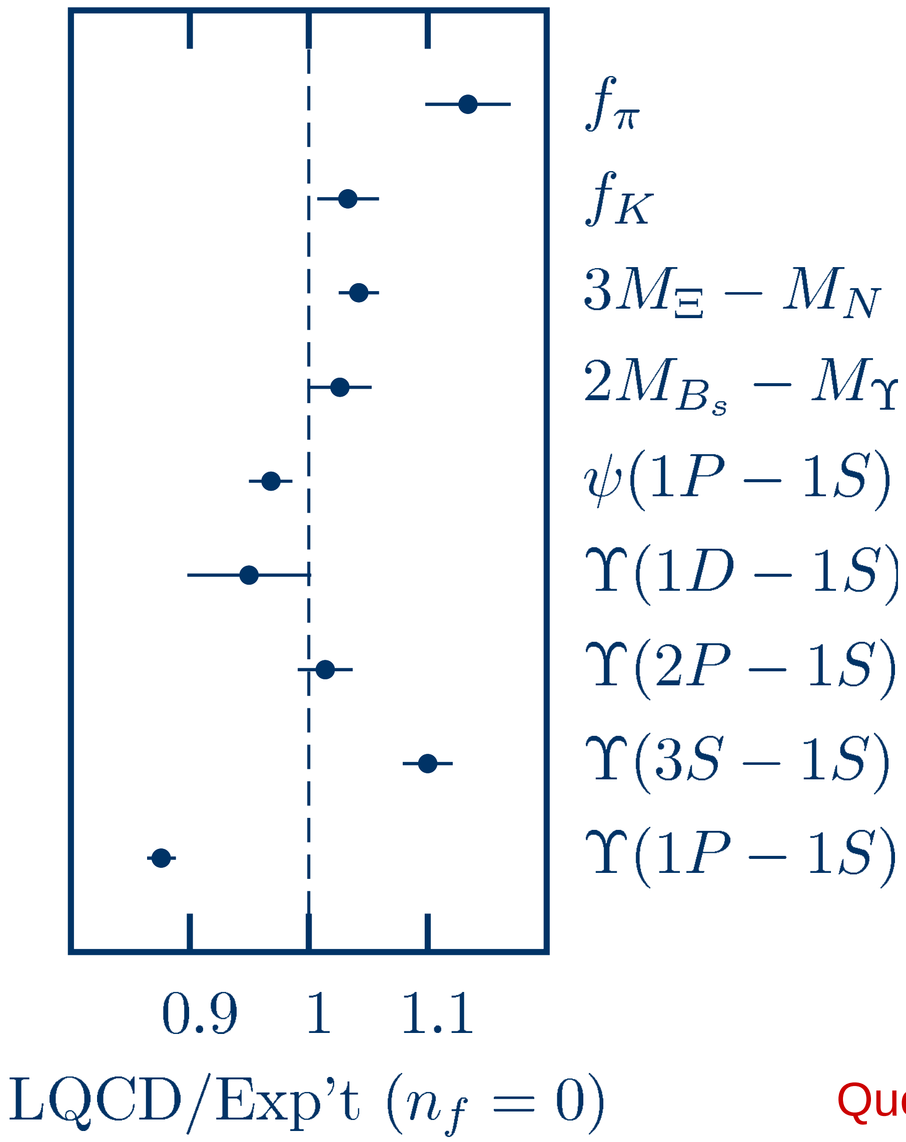
Physicists at Cornell, Fermilab, Simon Fraser, Glasgow, Illinois, & Ohio State starting working on them too. $\Rightarrow$ `hep-lat/0304004`

As each collaboration did its own work, we began to realize that the simulations were working in the way that had been long expected:

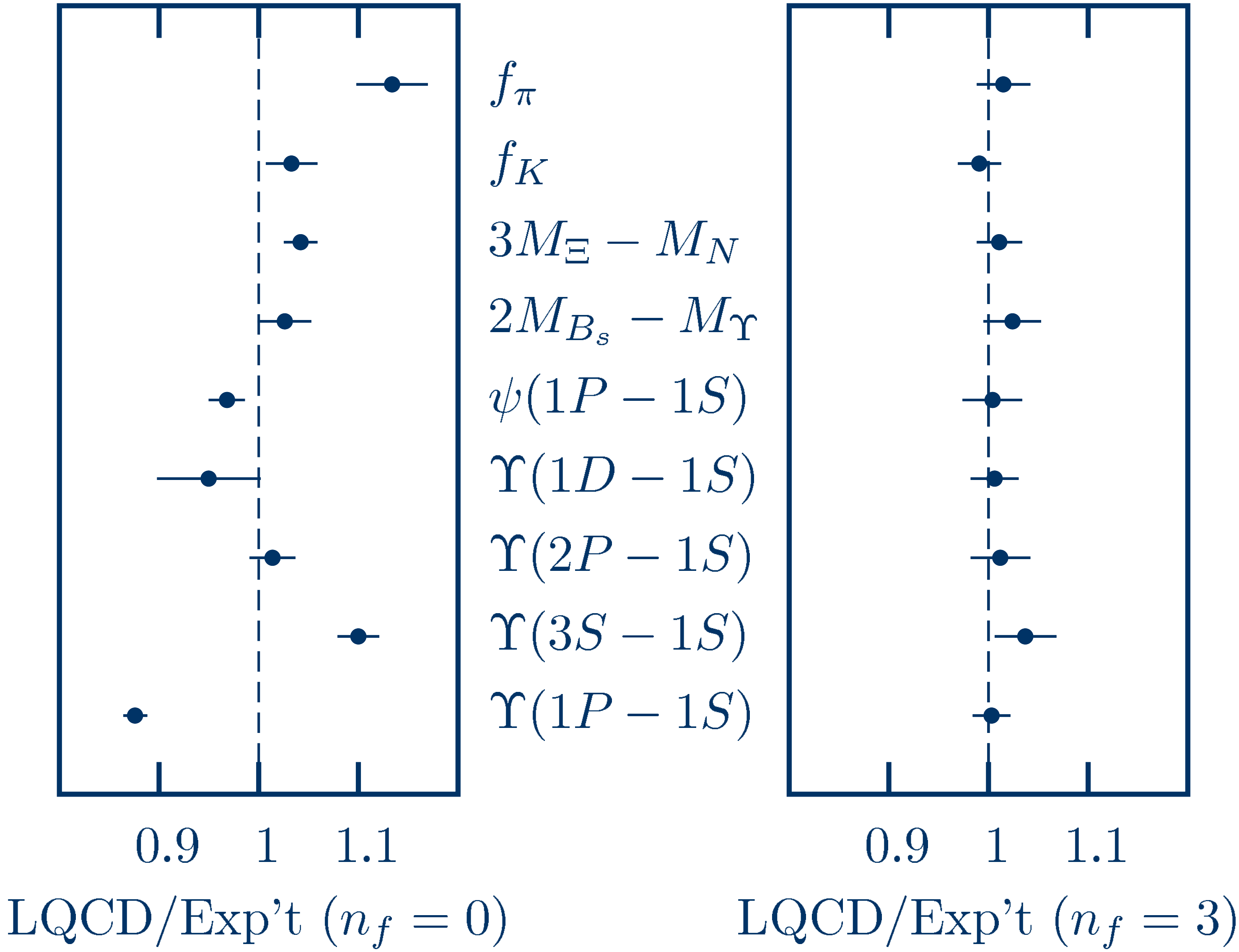
Set $1+4$ free parameters:	$a(g_0^2)$;	m_{0l}, m_{0s}, m_{0c}, m_{0b}
with $1+4$ meson masses:	$m_{\Upsilon(2S)} - m_{\Upsilon(1S)}$;	m_π^2, m_K^2, m_{D_s}, $m_{\Upsilon(1S)}$.

Compute several other properties of light mesons and baryons, charmonium, and B_s—all in all a wide variety of probes of the QCD scale.

Compare with experiment.



Quenched, with parameters fixed.


f_π
f_K
$3M_\Xi - M_N$
$2M_{B_s} - M_\Upsilon$
$\psi(1P - 1S)$
$\Upsilon(1D - 1S)$
$\Upsilon(2P - 1S)$
$\Upsilon(3S - 1S)$
$\Upsilon(1P - 1S)$
0.9
1
1.1
LQCD/Exp't $(n_f = 0)$
0.9
1
1.1
LQCD/Exp't $(n_f = 3)$

High-Precision Lattice QCD Confronts Experiment

C. T. H. Davies,[1] E. Follana,[1] A. Gray,[1] G. P. Lepage,[2] Q. Mason,[2]
M. Nobes,[3] J. Shigemitsu,[4] H. D. Trottier,[3] and M. Wingate[4]
(HPQCD and UKQCD Collaborations)

C. Aubin,[5] C. Bernard,[5] T. Burch,[6] C. DeTar,[7] Steven Gottlieb,[8] E. B. Gregory,[6]
U. M. Heller,[9] J. E. Hetrick,[10] J. Osborn,[7] R. Sugar,[11] and D. Toussaint[6]
(MILC Collaboration)

M. Di Pierro,[12] A. El-Khadra,[13] A. S. Kronfeld,[14] P. B. Mackenzie,[14] D. Menscher,[13] and J. Simone[14]
(HPQCD and Fermilab Lattice Collaborations)

[1] *Department of Physics and Astronomy, University of Glasgow, Glasgow, United Kingdom*
[2] *Laboratory for Elementary-Particle Physics, Cornell University, Ithaca, New York 14853*
[3] *Physics Department, Simon Fraser University, Vancouver, British Columbia, Canada*
[4] *Physics Department, The Ohio State University, Columbus, Ohio 43210*
[5] *Department of Physics, Washington University, St. Louis, Missouri 63130*
[6] *Department of Physics, University of Arizona, Tucson, Arizona 85721*
[7] *Physics Department, University of Utah, Salt Lake City, Utah 84112*
[8] *Department of Physics, Indiana University, Bloomington, Indiana 47405*
[9] *American Physical Society, One Research Road, Box 9000, Ridge, New York 11961-9000*
[10] *University of the Pacific, Stockton, California 95211*
[11] *Department of Physics, University of California, Santa Barbara, California 93106*
[12] *School of Computer Science, Telecommunications and Information Systems, DePaul University, Chicago, Illinois 60604*
[13] *Physics Department, University of Illinois, Urbana, Illinois 61801-3080*
[14] *Fermi National Accelerator Laboratory, Batavia, Illinois 60510*

hep-lat/0304004

Gold-Plated Quantities

The 5 mass (splittings) used to adjust the bare parameters and the 9 test quantities are all, in a sense, "gold-plated."

(*i*) 1 hadron in the initial state and 0 or 1 hadron(s) in the final state.
(*ii*) Hadrons either stable (π, K, N, Ξ, D_s, B_s) or narrow and well below threshold (ψs, Υs).

Particles that decay (*e.g.*, ρ, ϕ, Δ, $\psi(2S)$, $\Upsilon(4S)$) or two-particles states (*e.g.*, $\pi\pi$ in $K \to \pi\pi$) are more difficult to handle cleanly.

It is also important to control the chiral extrapolation—relevant for K and π physics (and B and D). More on this later.

Survey of Lattice Fermions

Fermion loops are the most computationally demanding part of lattice QCD—$\det M$.

Fermion propagators second-most—$M^{-1}S$.

There are several methods, with various theoretical and computational advantages and disadvantages: Wilson, staggered, domain-wall, overlap (Neuberger).

Can be traced back to the Nielsen-Ninomiya Theorem: there is an obstacle to maintaining *ultra*-locality, chiral symmetries, sensible time-evolution, while avoiding species doubling.

N.B., ultra-locality needed to define a Hamiltonian for $a \neq 0$.

Costs of Dynamical Fermions

Studies of algorithms for (improved) Wilson fermions suggest

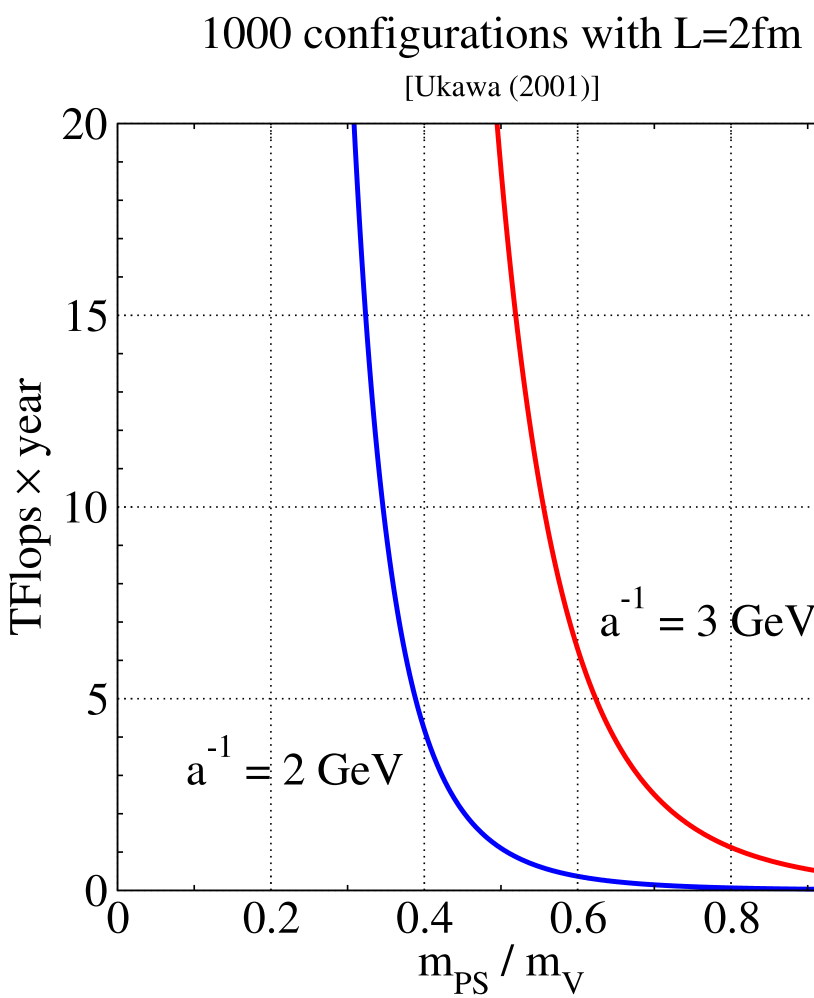
$$\texttt{cost} \propto \left(\frac{m_{\rm PS}^2}{m_{\rm V}^2}\right)^3 L^5\, a^{-7}$$

The Berlin Wall.

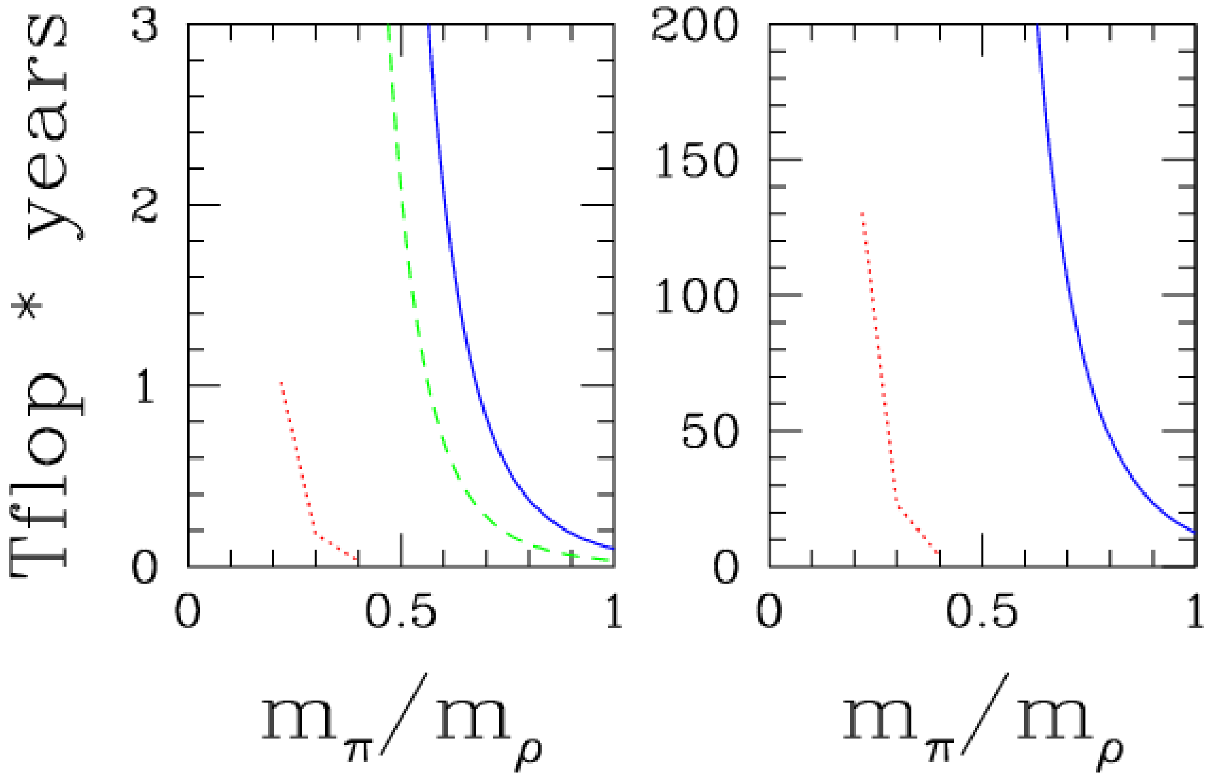
Phenomenology, not data.

Domain-wall and overlap are both much, much slower.

Plots from K. Jansen.



Staggered Quarks are Faster!



Wilson

Wilson/3

$a = 1/11$ fm

measured

$a = 1/22$ fm

extrapolated $\propto a^{-7}$

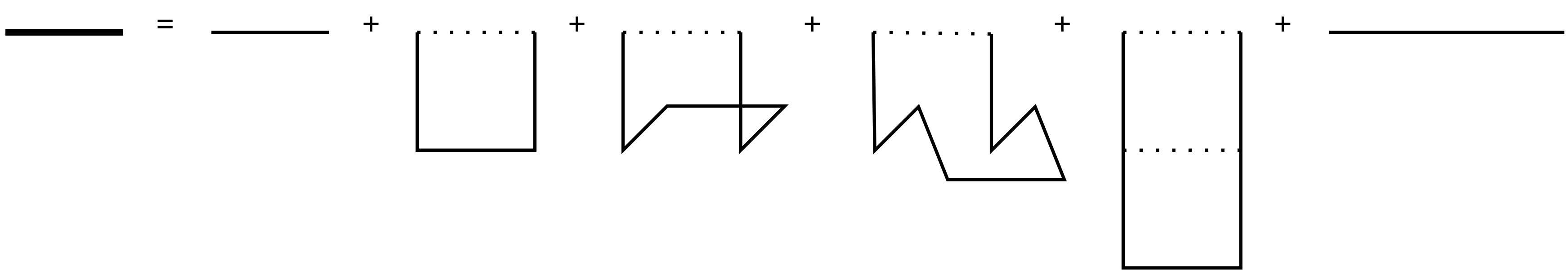
Staggered fermions provide the only method that is fast enough to reach small enough masses for light quarks (loops and valence quarks) on current computers.

Problems with Staggered Fermions

Staggered fermions suffer from a few problems: the central one is that one lattice fermion field produces 4 species (or tastes).

A side-effect until a few years ago was large discretization errors (formally of order a^2). Traced to taste-changing interactions.

Orginos and Toussaint found an empirical way to remove them: Fat7 (still $O(a^2)$).



Lepage added a term to reduce discretization effects to $O(\alpha_s a^2, a^4)$: Asqtad action.

From 4 Tastes to 1

Staggered fermions are supposed to yield 4 Dirac fermions in the continuum limit. How do we arrive at 1 or 2 flavors?

Fermion loops come from $\det M$, where M is a discretization of $\not{D} + m$. In the fermion-loop algorithm, one simply takes $(\det M)^{n_f/4}$.

Does $(\det M)^{n_f/4} = \det(M^{n_f/4})$?

$$M = \begin{pmatrix} \tilde{M} & & & \\ & \tilde{M} & & \\ & & \tilde{M} & \\ & & & \tilde{M} \end{pmatrix} + a\mathcal{N} = \mathcal{M} + a\mathcal{N}, \qquad \mathcal{N} \text{ not block diagonal}$$

$$(\det M)^{n_f/4} = (\det \tilde{M})^{n_f} \left[1 + \tfrac{1}{4} n_f a \, \mathrm{tr}(\mathcal{N}\mathcal{M}^{-1})\right],$$

Do the terms $a^2 \mathcal{M}^{-2}$ (and their higher order siblings) spoil locality when $a \longrightarrow 0$?

To all orders in perturbative QCD, quark loops are treated correctly.

Further analysis is not so straightforward.

Explicit constructions of the 4 tastes are notationally voluminous.

The separation is clean (and local) for free fields, but muddied when gauge fields are introduced.

The Asqtad action was specifically designed to reduce taste-changing interaction, denoted here as $\mathcal{N}$.

At present there is circumstantial evidence: the details of m_{PS} and f_{PS}.

For me it is compelling enough to believe that this method should be pursued.

The Problem of Light Quarks

The algorithms literally hit a wall when

$m_{\mathrm{PS}} < 0.7 m_{\mathrm{V}}$	Wilson (and SW)
$m_{\mathrm{PS}} < 0.3 m_{\mathrm{V}}$	staggered

or

$m_q < 0.6 m_s$	Wilson (and SW)
$m_q < 0.1 m_s$	staggered

In Nature $m_d = 0.04 m_s$ and m_u is about 3 times smaller still.

Extrapolate $m_q \to 0$ (nearly), called the chiral extrapolation.

Often the largest source of systematic uncertainty (and frequently underestimated in quenched calculations).

Chiral Perturbation Theory

Chiral perturbation theory (χPT) allows us to describe the dependence of hadronic quantities on the masses of light pseudoscalar mesons:

$$A = A_0 + A_1(\mu)\frac{m_\pi^2}{(4\pi f_\pi)^2} + A_\chi \frac{m_\pi^2}{(4\pi f_\pi)^2}\ln(m_\pi^2/\mu^2)$$

The last term is called a “chiral log”. $f_\pi = 132$ MeV

Really the limiting behavior of the function obtained from 1-loop integrals.

Something non-analytic in $m_\pi^2 \propto m_q$ always appears; not always a log

e.g., $m_\pi^3 = (m_\pi^2)^{3/2}$ in masses of heavy hadrons.

Replace m_π with m_{PS}, the mass as calculated in the simulation, and fit.

Chiral symmetry constrains A_χ to something known or “knowable.” It is not a completely free parameter.

Chiral Extrapolations of f_π and f_K

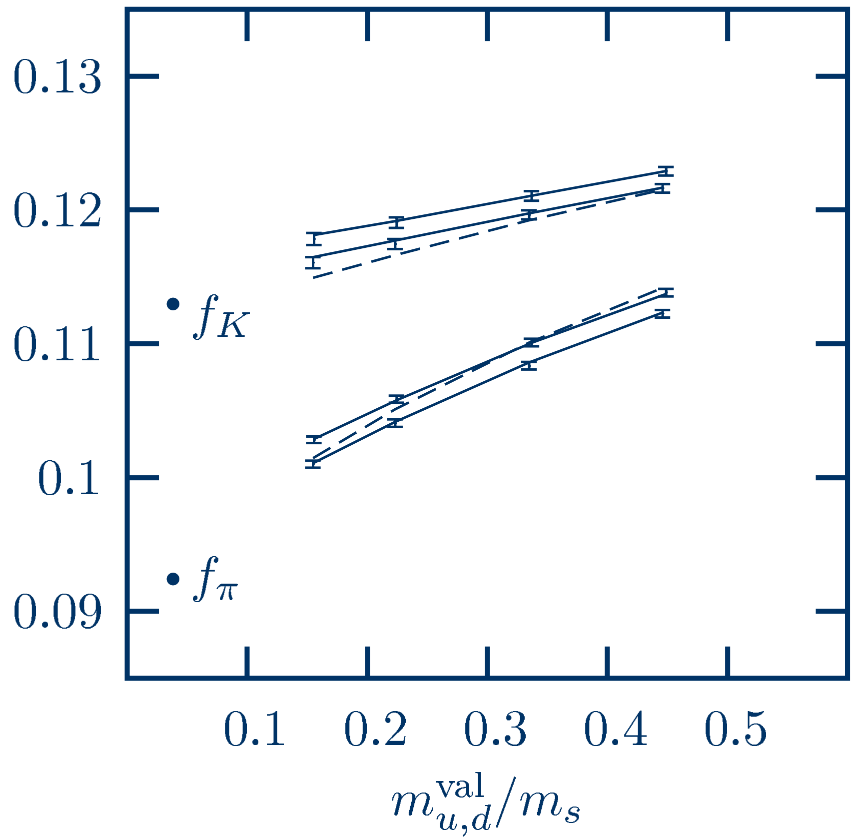
Dots at 0.04 are experiment values.

Error bars are lattice QCD, with two runs with different m_q^{sea}.

Linear extrapolation (by eye) gets close.

Chiral log fits (dashed curves) at fixed a get closer.

Chical log fit, now correcting for $O(a^2)$, gets even closer. (On the ratio plot.)



An even more remarkable analysis [Aubin & Bernard] follows.

χPT for Taste-Symmetry Violation

WARNING: this gets complicated!

For 4 species the taste symmetry group should be SU(4)$\times$SU(4).

Discretization break it to $\Gamma_4 \times$U(1), leading to more non-analytic contributions in χPT.

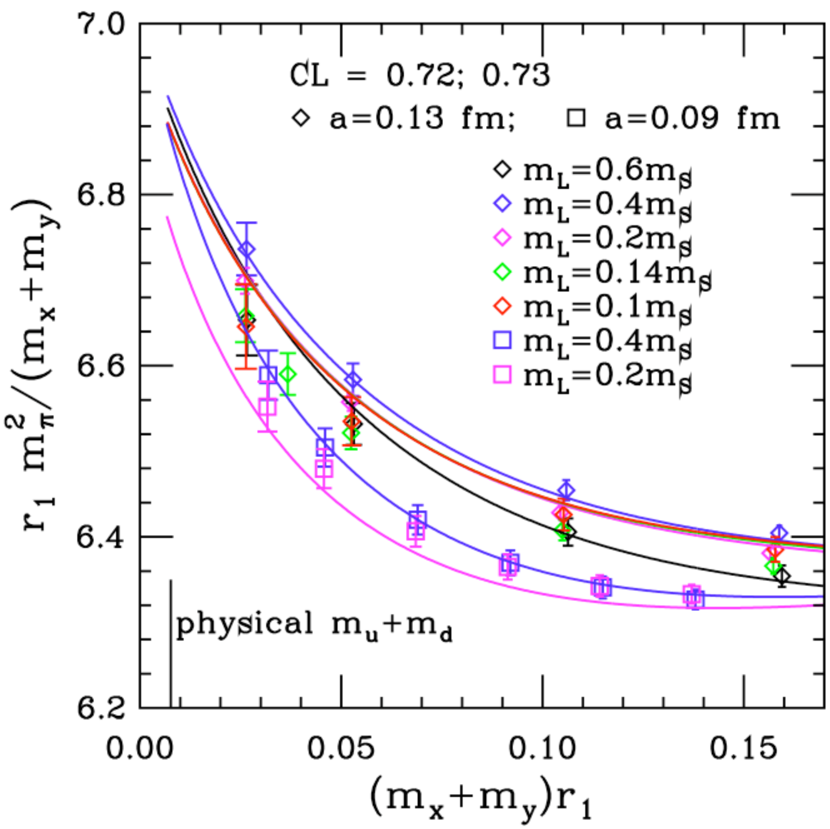
Also possible to account for $(\det M)^{n_f/M}$ in χPT: SU$(4|4-n_f)\times$SU$(4|4-n_f)$.

And possible to account for $m_q^{\text{valence}} \neq m_q^{\text{sea}}$.

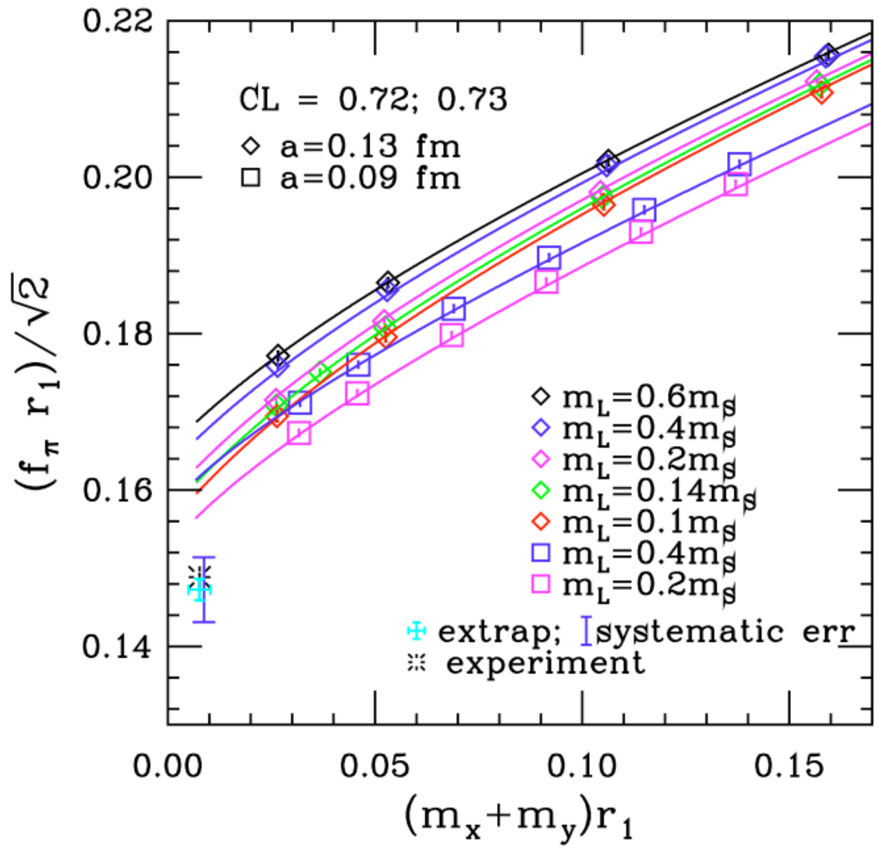
Aubin and Bernard put this all together to obtain unpresentable formulas.

Statistical precision of MILC is good enough to fit them.

χPT with Violations of Taste Symmetry



one fit



one fit

$B \to D^* l\nu$, $|V_{cb}|$, and $\mathcal{F}(1)$

$$\frac{d\Gamma}{dw} \propto |V_{cb}|^2 |\mathcal{F}(w)|^2$$

where the form factor $\mathcal{F}(w)$ is obtained from vector *and* axial-vector $B \to D^*$ transitions.

At zero recoil, $w \to 1$, $\mathcal{F}$ reduces to a certain axial-vector form factor, h_{A_1}. Moreover, heavy-quark symmetry [Luke's Theorem] forbids $1/m_Q$ corrections to the heavy-quark limit.

The variable $w = v_B \cdot v_D$ is the velocity transfer, related to q^2.

A couple of years ago, we figured out how to expoit the HQET interpretation of lattice gauge theory to obtain the corrections $\mathcal{F} - 1$ from numerical simulations.

Strictly speaking, the D^* is not one of our gold-plated mesons. It decays $D^* \to D\pi$.

However, it is just above threshold, and the threshold is pushed away for feasible light quark masses.

More importantly, all uncertainties (including quenching) scale as $\mathcal{F}(1) - 1$.

So $\mathcal{F}(1)$, if not gold-plated, is sterling sliver.

$$\mathcal{F}(1) = 0.913^{+0.024}_{-0.017} \pm 0.016^{+0.003}_{-0.014}{}^{+0.000}_{-0.016}{}^{+0.006}_{-0.014}$$

with uncertainties from statistics and fitting, HQET matching, lattice-spacing effects, chiral extrapolation, and quenching [Hashimoto *et al.*, hep-ph/0110253].

$B \to \pi l \nu$, $|V_{ub}|$, and $f_+(E_\pi)$

$$\frac{d^2\Gamma}{dE_l dE_\pi} \propto |V_{ub}|^2 |f_+(E_\pi)|^2$$

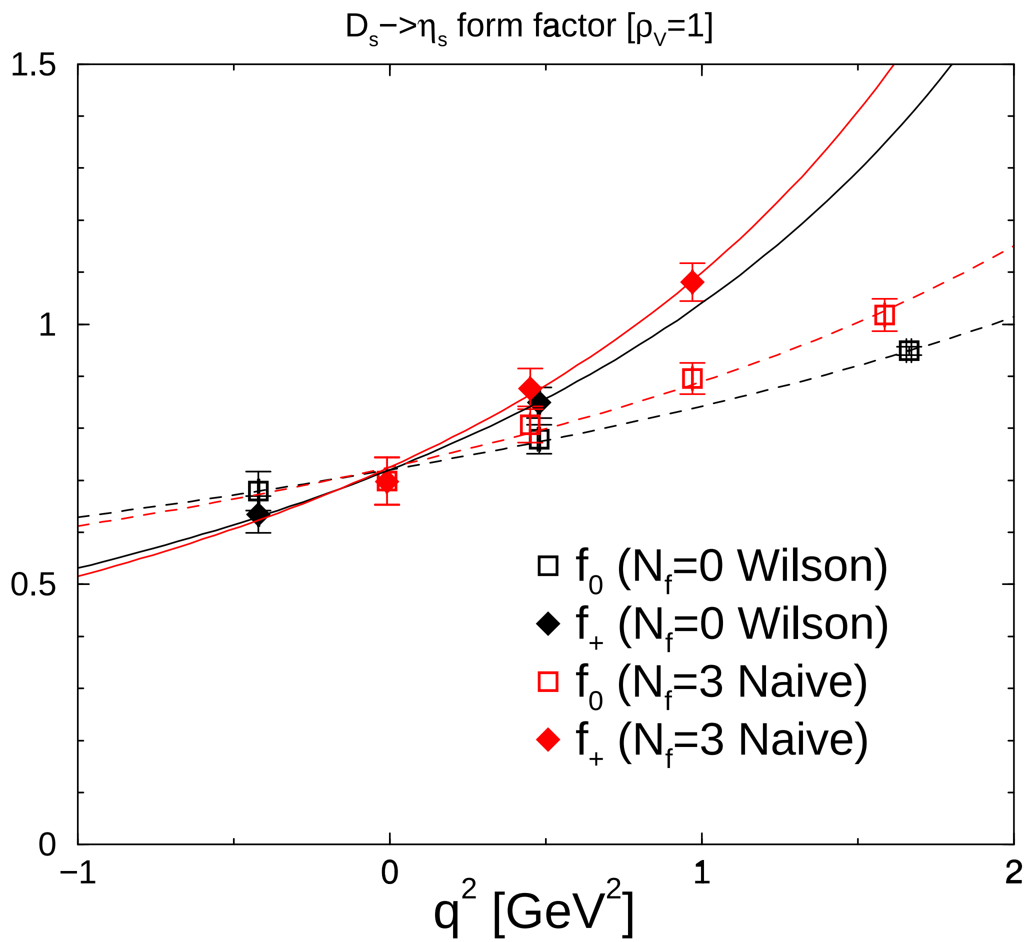
where the form factor is obtained from vector $B \to \pi$ transitions.

It is worth noting that the lepton energy dependence is completely known. For determining $|V_{ub}|$ it is not necessary to integrate over all E_l. It is enough to integrate over experimental acceptance.

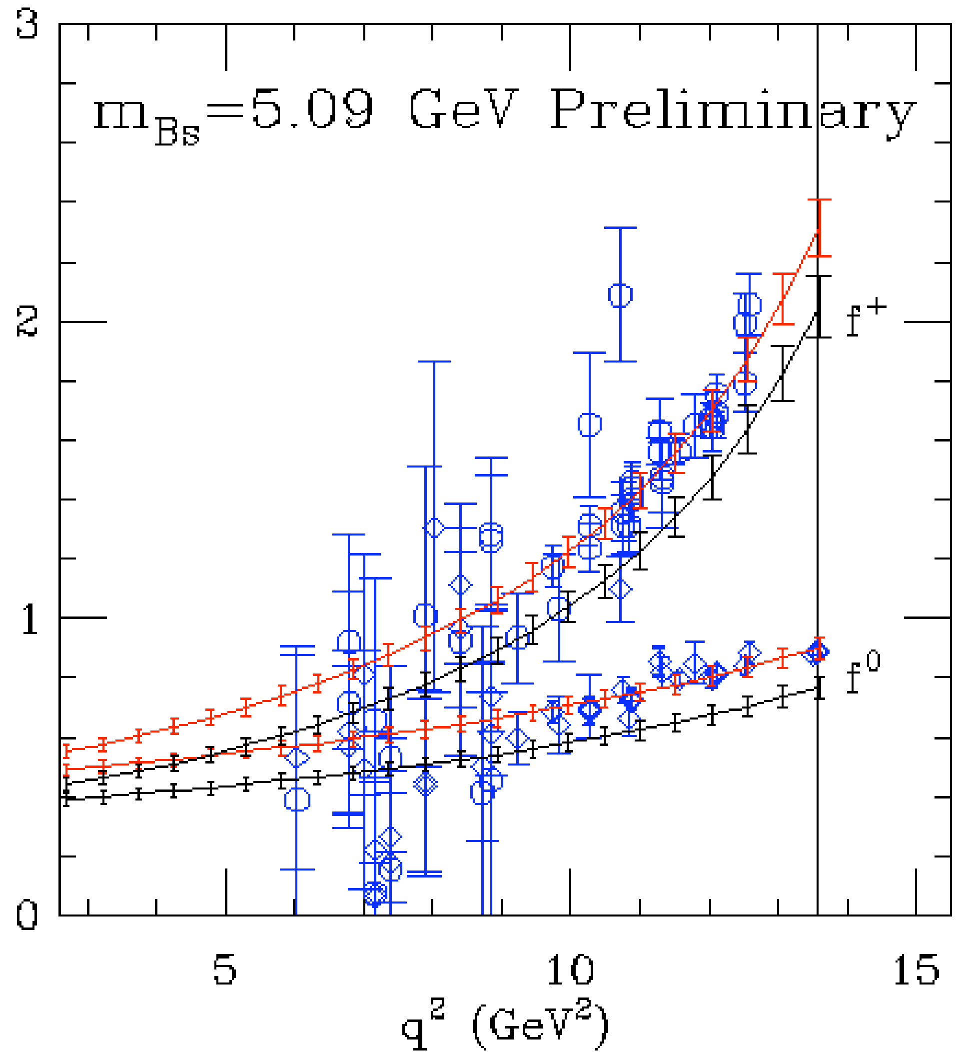
The variable $E_\pi = v \cdot p_\pi$ is the pion energy in the rest frame of the B meson.

In the quenched approximation there is good (but not excellent) agreement on f_+ between UKQCD, Fermilab, APE, and JLQCD. Agreement on f_0 is poor.

Chiral extrapolations not easy and not done especially well. The is now better guidance from χPT [Becirevic et al.].



D_s−>η_s form factor [ρ_V=1]
1.5
1
0.5
0
−1
0
1
2
q^2 [GeV^2]
f_0 (N_f=0 Wilson)
f_+ (N_f=0 Wilson)
f_0 (N_f=3 Naive)
f_+ (N_f=3 Naive)


m_{Bs}=5.09 GeV Preliminary
f^+
f^0
0
1
2
3
5
10
15
q^2 (GeV^2)

Δm_q, $|V_{tq}|$, and ξ

We saw in several lectures that the oscillation frequency

$$\Delta m_q \propto |V_{tq}|^2 \tfrac{8}{3} m_{B_q}^2 f_{B_q}^2 B_{B_q}$$

where the matrix element of the $\Delta B = 2$ operator is written in a peculiar way.

An obvious strategy to reduce the theoretical uncertainties is to take the ratio

$$\frac{\Delta m_s}{\Delta m_d} \propto \frac{|V_{ts}|^2}{|V_{td}|^2} \frac{m_{B_s}^2}{m_{B_d}^2} \xi^2, \qquad \xi = \frac{f_{B_s}\sqrt{B_{B_s}}}{f_{B_d}\sqrt{B_{B_d}}}$$

The experimental precision is percent level. (Δm_s is this precise as soon as it is resolved.)

It was argued for many years that ξ was known at the 5% level: $\xi = 1.15 \pm 0.5$, including an estimate of the quenching error.

This value and error bar, especially the notion that a drastic cancellation of the uncertainty, propagated to the experimental community.

This despite warnings from Booth [1994] and Sharpe&Zhang [1995] that $\xi - 1$ could deviate, in the quenched approximation, by as much as 100%.

This disparity led Sinéad Ryan and me to look at the arguments again.

Uncertainties in $f_B^2 B_B$ can come from several sources. Most do cancel, at least to some extent: statistics, lattice spacing effects, heavy-quark effects

$$\xi = \frac{f_{B_s}\sqrt{B_{B_s}}}{f_{B_d}\sqrt{B_{B_d}}}$$

even, arguably, quenching effects at the scale Λ_{QCD}.

This leaves uncertainty from the difference in the light quark masses: m_s vs. $m_l \to m_d$.

The central value (~ 1.15) came from a linear extrapolation in $r = m_l/m_s$, with $r > 0.5$.

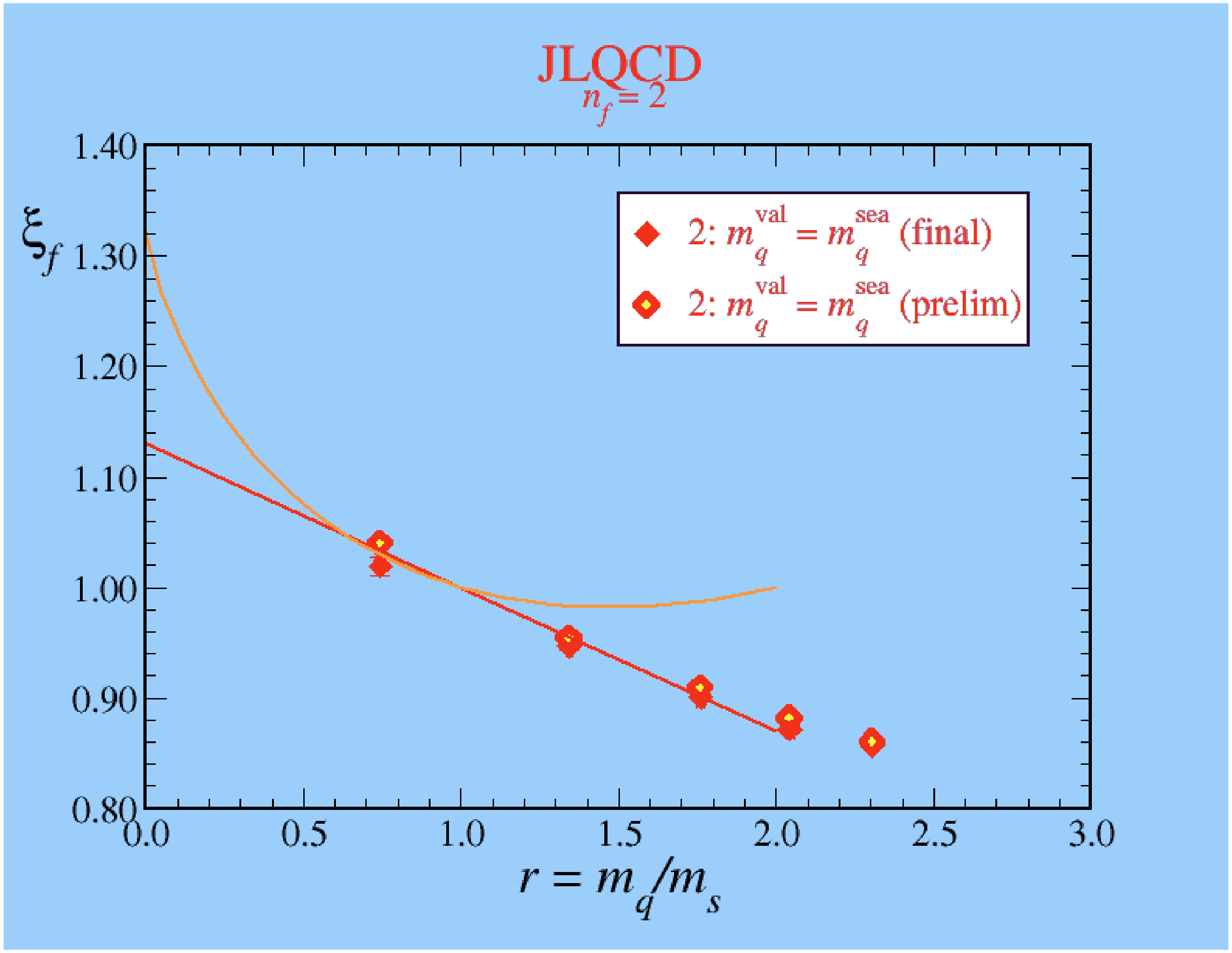
As $m_l \to m_d = m_s/24$ this is certainly not correct: chiral perturbation theory says there must be a term $m_\pi^2 \ln m_\pi^2$, and $m_\pi^2 \propto m_l$, which has curvature.

We tried a different strategy: use the same lattice data, but interpret them as a determination of the analytic term in χPT. Then follow the χPT curve with chiral log.

Needs some phenomenology: the B-B^*-π coupling. We assumed a large range around the measured D-D^*-π coupling.

Since then, the two most interesting developments are JLQCD's calculations of f_B and B_B [hep-ph/0307039], and preliminary calculations of f_B on the MILC ensemables.

$$\xi = \begin{cases} 1.30 \\ \qquad\qquad ??? \\ 1.13 \end{cases}$$



Best result

w/o staggered

light quarks

$$\xi = \begin{cases} 1.30 \\ \quad\quad ??? \\ 1.13 \end{cases}$$

Result with

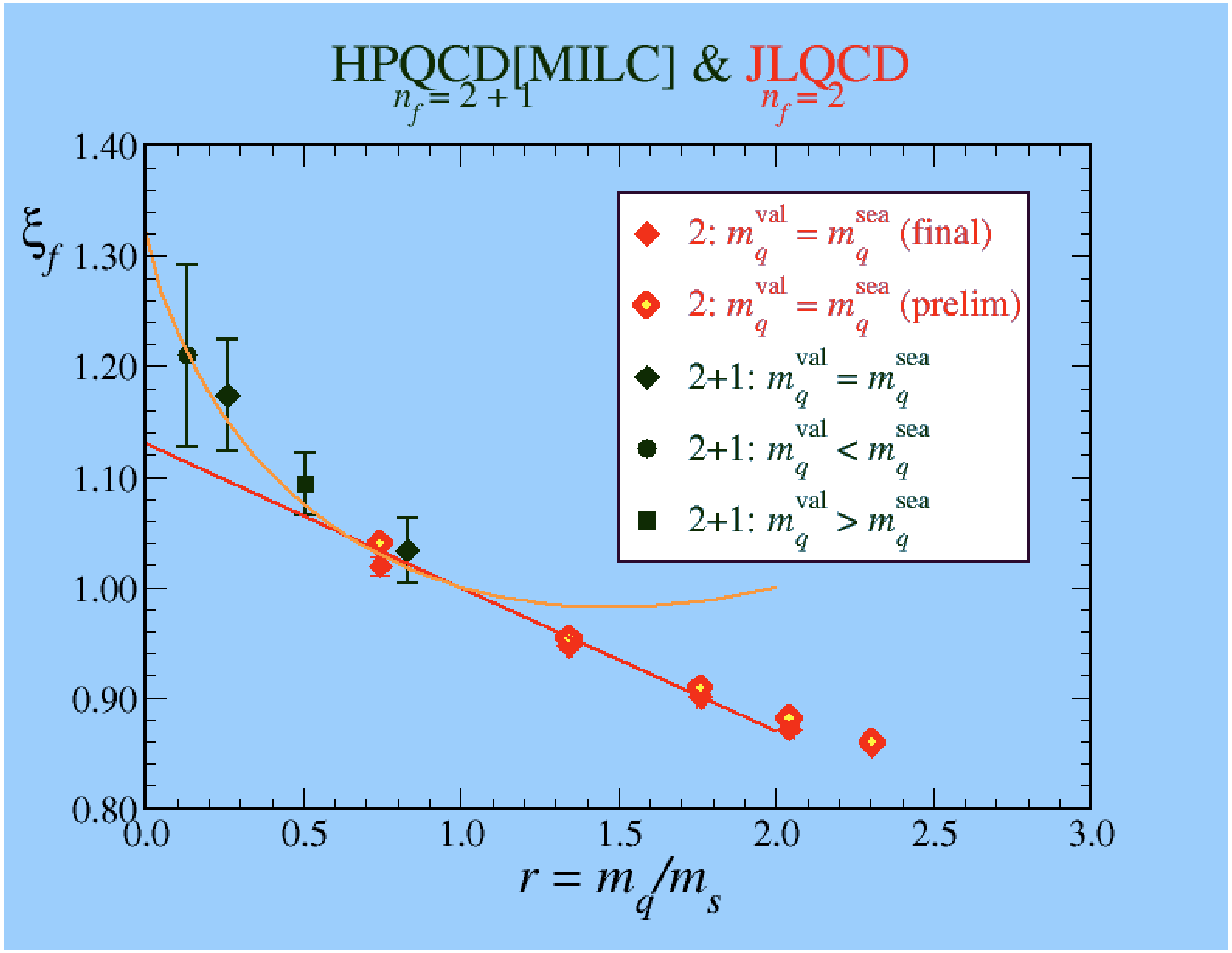
Asqtad $2+1$

[Wingate]

Best result

w/o staggered

light quarks



Outlook and Further Tests

The recent results with improved staggered quarks are very promising.

The goals are, however, extremely ambitious: uncertainties not merely small but robust enough to support a claim of new phenomena in B physics (if indeed it's there).

Any numerical simulation is, in the end, fairly inscrutable to outsiders. Are there any predictions? Any tests?

There are several things that should be easy for us (and are in progress), and, though unmeasured or poorly measured, will be measured well soon.

Decay constants and form factors of D and D_s mesons (coming from CLEO-c); the mass of the B_c (coming from CDF).

An especially intriguing test is as follows.

CLEO-c will measure $D \to l\nu$ and $D \to \pi l\nu$. The ratio

$$\frac{1}{\Gamma(D \to l\nu)} \frac{d\Gamma(D \to \pi l\nu)}{dE_\pi} \propto \left[\frac{|f_+(E_\pi)|}{f_D} \right]^2$$

is a direct test of non-perturbative QCD. The missing factor is simply kinematics. Couplings such as CKM and even G_F drop out.

Similarly $|f_+^{D\to K}(E_K)|/f_{D_s}$.

Next year I hope I can plot lattice QCD and (a few months later) overlay experiment.

If this test succeeds, we can note that the B form factors and decay constants have similar (perhaps smaller) systematics, and all these are gold-plated, in the sense given above.