Predictive Lattice QCD

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Fermilab

Preface

Title Deconstructed

Predictive Lattice QCD

QCD is quantum chromodynamics, the modern theory of the strong (nuclear) force. Quarks & gluons ⇒ hadrons.

Lattice QCD is a way to calculate long-distance properties with a lot of computing—O(10) Tflop-years' worth.

Any computational enterprise is more persuasive if it can **predict** something before it's been measured.

PC Clusters at Fermilab

Outline

- Introduction: the long and short of QCD.
- Reflection: Why are we here?
- Challenge: obstacles to lattice QCD.
- Success: numerical simulation + effective field theory.
- Predictions: calculations preceding measurements.
- Outlook: influences on flavor physics and beyond.

The Long & Short of QCD

QCD

- Quantum chromodynamics is part of the Standard Model.
- SU(3) gauge symmetry.
- Mathematically almost like QED, “just messier.”
- QCD possesses asymptotic freedom, so at short distances perturbation theory is accurate and quantitative.
- Chromodynamics is not like electrodynamics at all.

Lagrangian of QED, QCD

$$\mathcal{L}_{\mathrm{QED}} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \bar{e}(\not{D} + m_e)e$$

$$D^{\mu} = \partial^{\mu} + ieA^{\mu}$$

$$F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$$

U(1)

photon A_{μ}

electron e

$$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{4}F^{a}_{\mu\nu}F^{\mu\nu a} - \bar{q}_i(\not{D}_{ij} + m_q)q_j$$

$$D^{\mu}_{ij} = \partial^{\mu}\delta_{ij} + g t^{a}_{ij}A^{\mu a}$$

$$F^{a}_{\mu\nu} = \partial_{\mu}A^{a}_{\nu} - \partial_{\nu}A^{a}_{\mu} + g f^{abc}A^{a}_{\mu}A^{b}_{\nu}$$

SU(3)

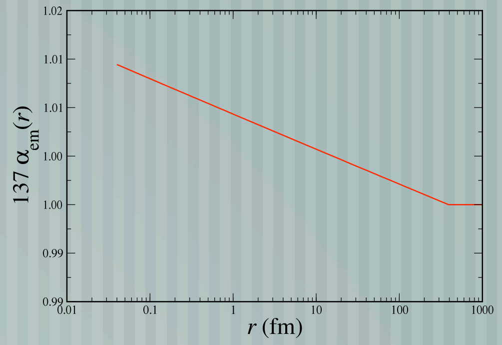
gluons A^{a}_{μ}

electron q_i

QCD compared to QED

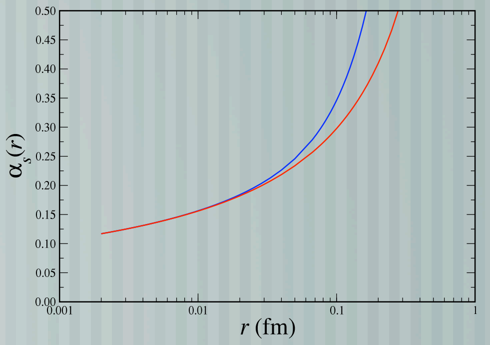
- In QED, virtual electron-positron pairs screen the bare charge:

$$F(r) = -\frac{\alpha(r)}{r^2}, \quad \alpha = \frac{e^2}{4\pi}$$

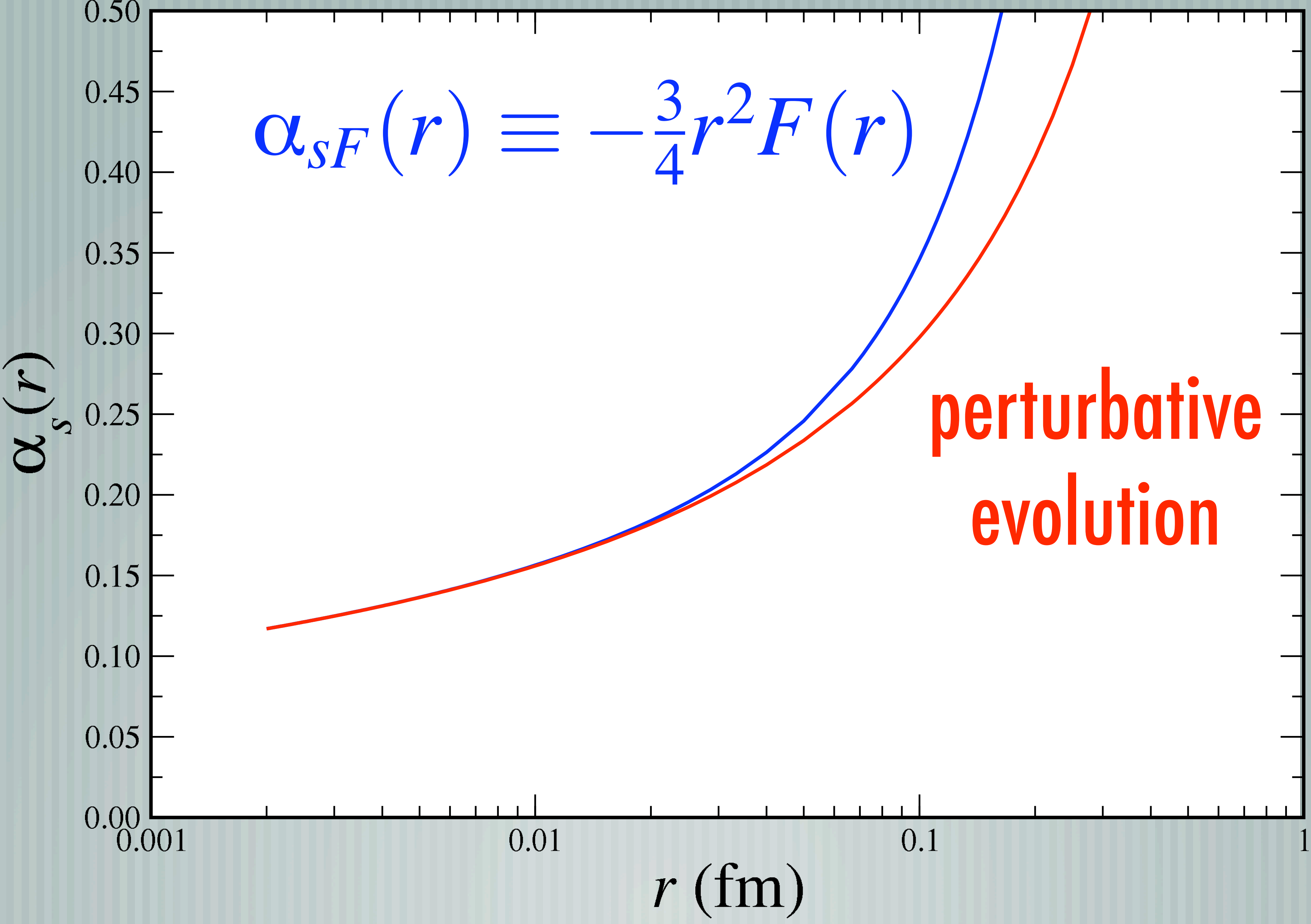


- In QCD, gluons, as well as quarks, carry color. They anti-screen:

$$F(r) = -\frac{4}{3}\frac{\alpha_s(r)}{r^2}, \quad \alpha_s = \frac{g^2}{4\pi}$$



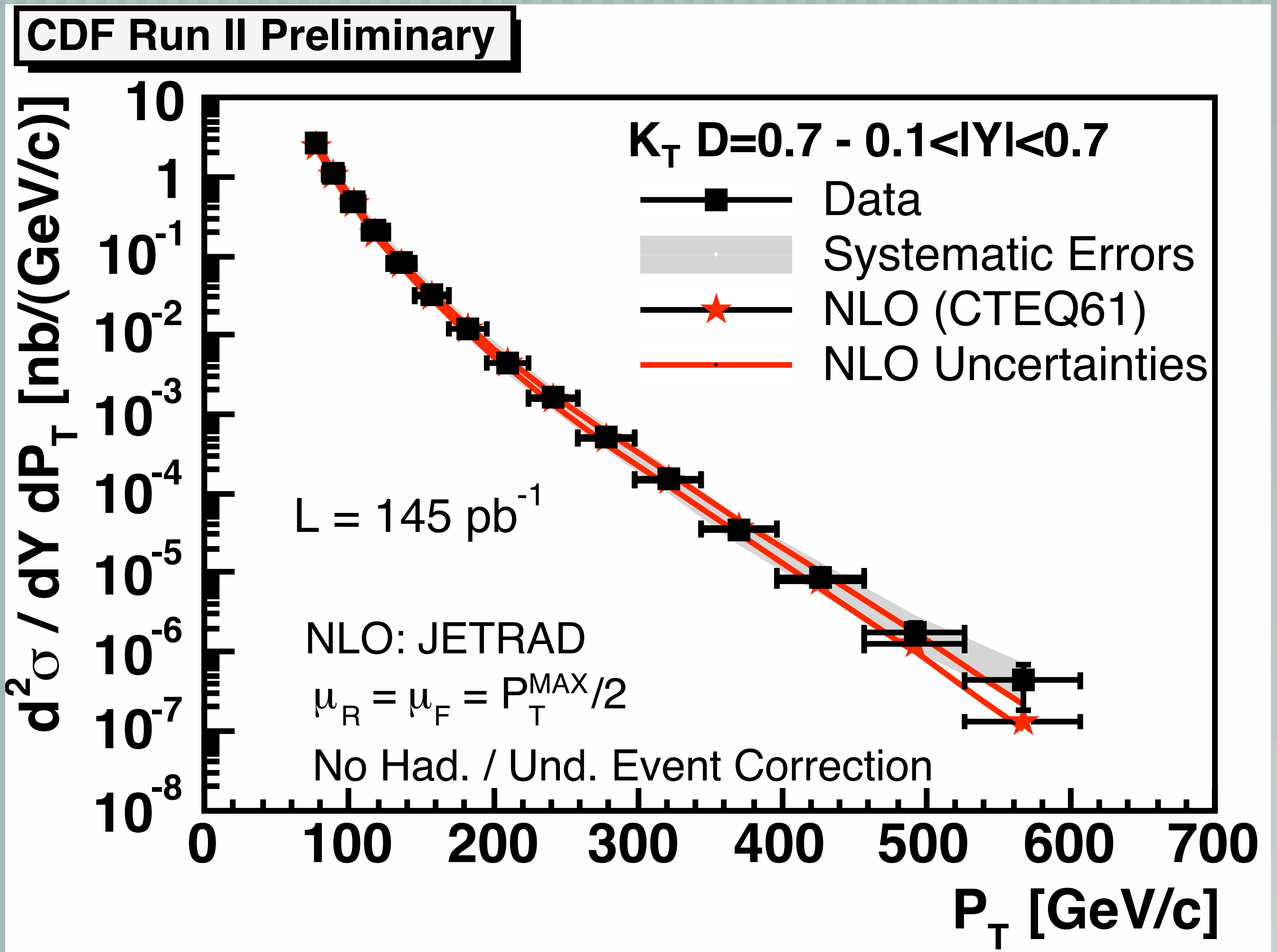
Asymptotic Freedom

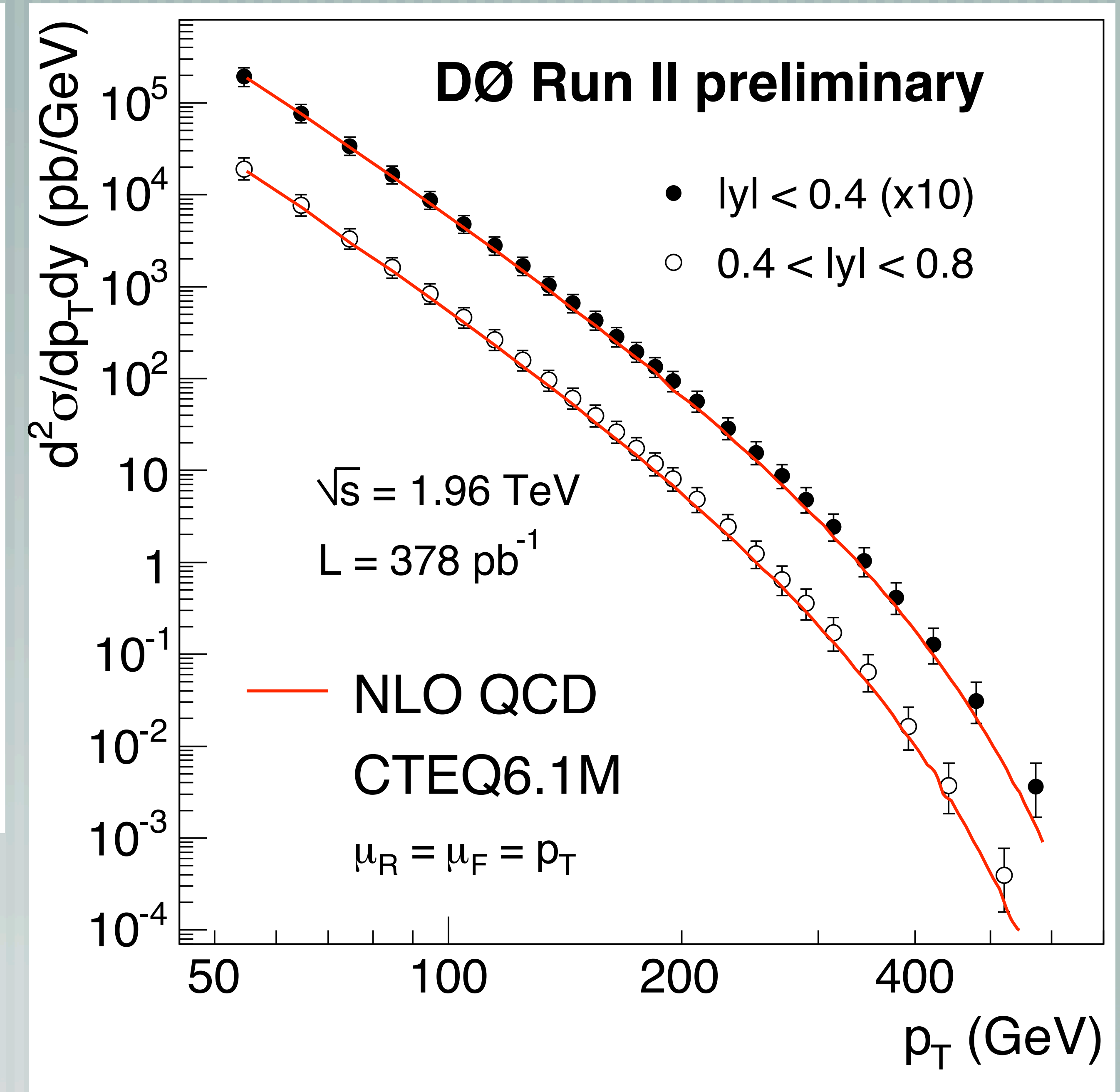


Asymptotic Freedom Rocks

- Because of asymptotic freedom, QCD is the “star” of the SM.
- It is theoretically consistent at all length scales
  - in contrast to the U(1) and Higgs sectors, where triviality says the theory must be replaced at some high scale.
- QCD’s short-distance behavior can be calculated accurately.
- Multi-GeV energies, multi-GeV temperatures, high densities.

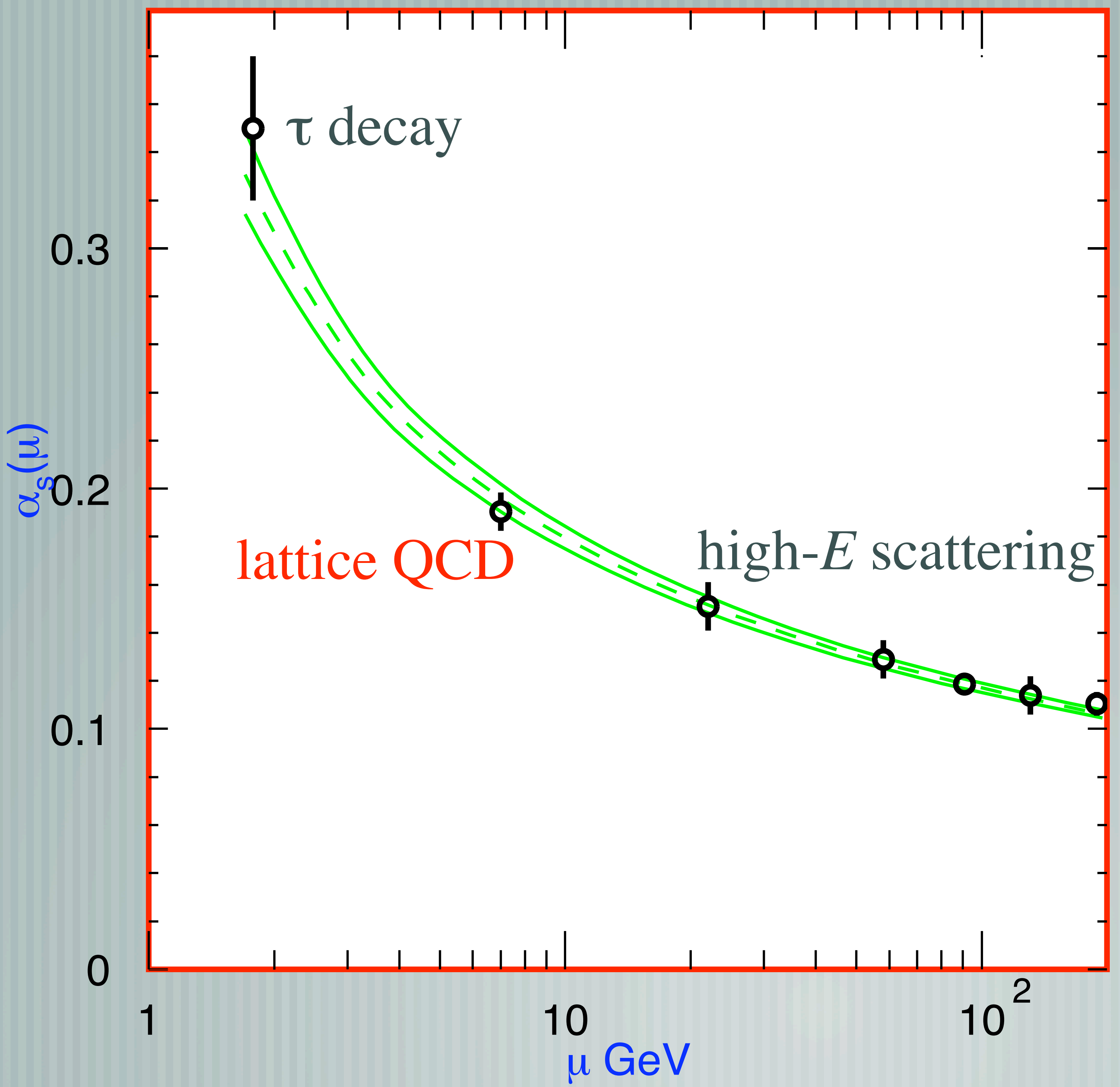
Single-jet Cross Section





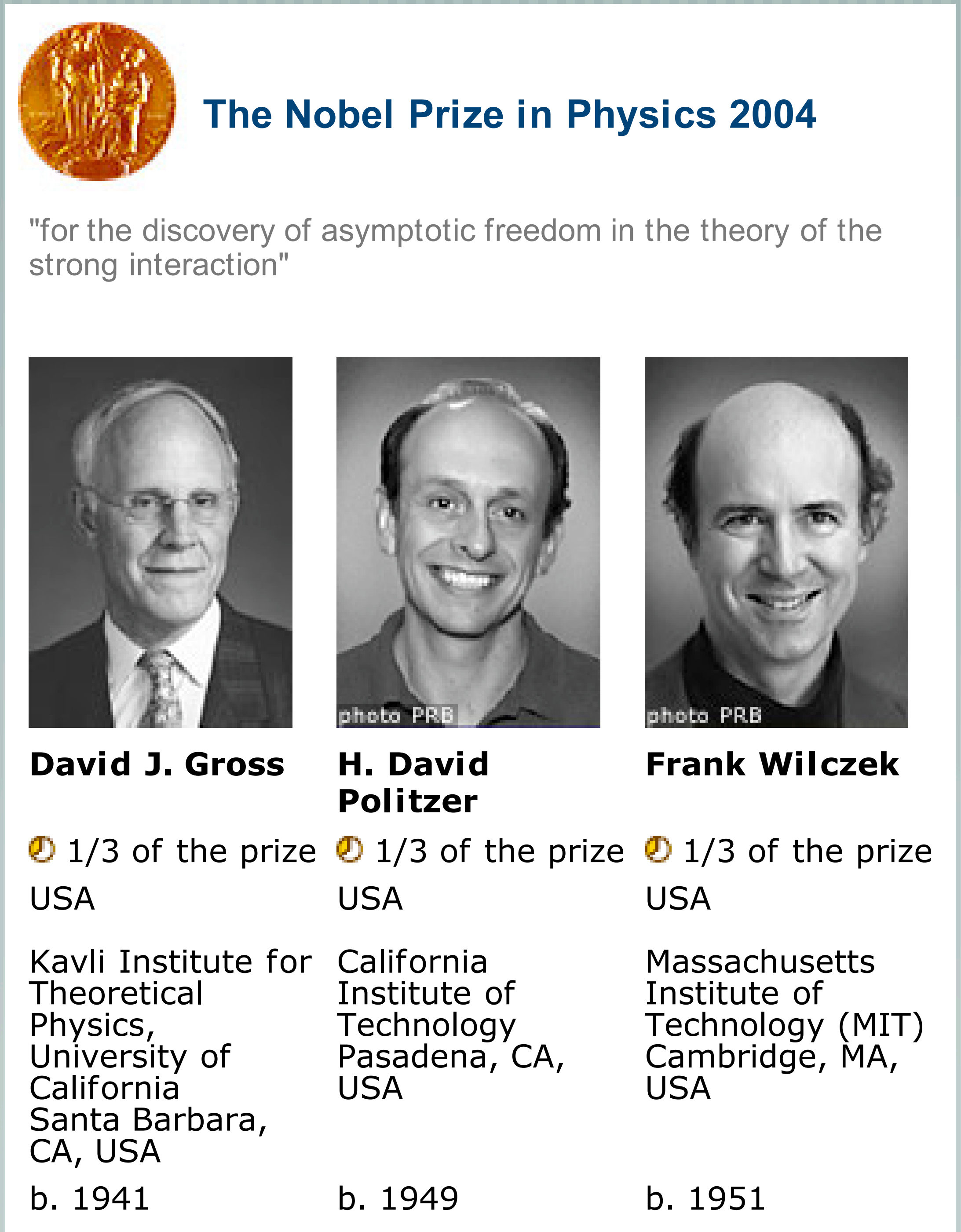
Agreement between data and NLO QCD PT over 8 orders of magnitude!

Running of α_s



PDG
Summary
Plot

Prize-worthy



The Nobel Prize in Physics 2004

"for the discovery of asymptotic freedom in the theory of the strong interaction"

David J. Gross	**H. David Politzer**	**Frank Wilczek**
◔ 1/3 of the prize	◔ 1/3 of the prize	◔ 1/3 of the prize
USA	USA	USA
Kavli Institute for Theoretical Physics, University of California Santa Barbara, CA, USA	California Institute of Technology Pasadena, CA, USA	Massachusetts Institute of Technology (MIT) Cambridge, MA, USA
b. 1941	b. 1949	b. 1951

Long Distances

- QCD is enormously successful at short distances, but ...
- ... at distances greater than $1\ \mathrm{fm} = 10^{-15}\ \mathrm{m}$, QCD forces become strong.
- Quantitatively, the perturbation series breaks down.
- Qualitatively, quarks and gluons are confined into hadrons.

- General-purpose tools—symmetry, unitarity, renormalization group, etc.—are not enough to calculate even the simplest properties of hadrons (masses, decay constants,...).
- What is needed is a definition of quantum field theory, including gauge theories like QCD, that is non-perturbative from the outset.
- With such a tool, we could solve old problems—like the calculation of the hadron spectrum ...
- ... and new problems in particle, nuclear, & astro physics.

On Beyond QCD

Standard Model of Elementary Particles

- Parts of the "Standard Model" are Laws of Nature
  - gauge symmetry $SU_c(3) \times SU_L(2) \times U_Y(1)$
  - gauge quantum numbers of quarks, leptons
- Parts are known, but not understood
  - EWSB: $SU_L(2) \times U_Y(1) \to U_{EM}(1)$
  - Flavor: fermion masses and mixing

Standard Quark Fields

two-component fields, with weak isopin ½

$$\begin{pmatrix} u \\ d \end{pmatrix}_L \quad \begin{pmatrix} c \\ s \end{pmatrix}_L \quad \begin{pmatrix} t \\ b \end{pmatrix}_L$$

which interact with *W*s

$$\left.\begin{matrix} u_R & c_R & t_R \\ d_R & s_R & b_R \end{matrix}\right\}$$

which do not

one-component fields, with weak isopin 0

Turn 9 into 6

69

- SU$_L$(2) symmetry is chiral and, thus, forbids quark masses
  - masses couple *L*eft and *R*ight
- Standard *Model* introduces one scalar doublet ϕ

$$y^u_{11}\bar{u}_R \begin{pmatrix}\phi^0 & \phi^+\end{pmatrix} \begin{pmatrix}u\\ d\end{pmatrix}_L + y^d_{11}\bar{d}_R \begin{pmatrix}\phi^- & \phi^{0*}\end{pmatrix} \begin{pmatrix}u\\ d\end{pmatrix}_L + \text{h.c}$$

- Electroweak symmetry breaking: $\langle\phi^0\rangle \neq 0$

- Also have (and all other combos)

$$y_{13}^{u}\bar{u}_R \left(\phi^0 \;\; \phi^+\right) \begin{pmatrix} t \\ b \end{pmatrix}_L + y_{13}^{d}\bar{d}_R \left(\phi^- \;\; \phi^{0*}\right) \begin{pmatrix} t \\ b \end{pmatrix}_L + \text{h.c.}$$

- So, as well as quark masses, these interactions lead to all sorts of generation-changing interactions.
- Provides the Standard source of CP violation.
- We know only that something like this happens; we do not know if the details are so simple.

Masses and CKM

- Masses
  - $m_u < m_d;\ m_c > m_s;\ m_t > m_b.$
- Cabibbo-Kobayashi-Maskawa (CKM) matrix
  - $V = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$ complex elements violate CP

Why are we here?

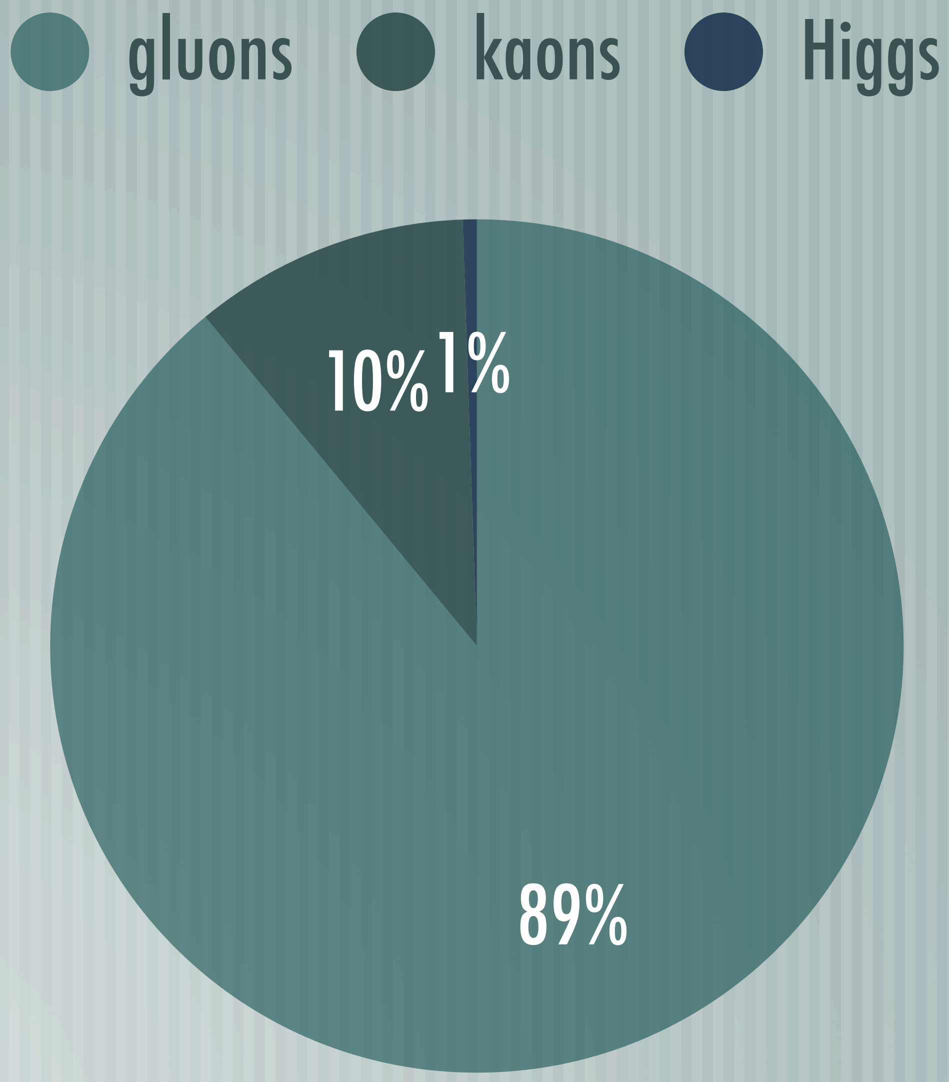
- Several mysteries in the microscopic world ...
  - electroweak symmetry breaking
  - (full) origin of CP violation
  - pattern of quark masses
- ... without which we cannot exist.
- Hence, we want to study the microscopic couplings of quarks.

Where are the quarks?

- Alas, the strong interactions are, well, too strong.
- Experiments do not detect quarks, they detect hadrons.
- To “measure” quark properties, theorists have to
  - understand why (quark confinement)
  - calculate effects of the strong interactions

Origin of Mass

Almost all the mass of ordinary matter comes from the chromodynamic energy of gluons and quarks whizzing around inside protons and neutrons.

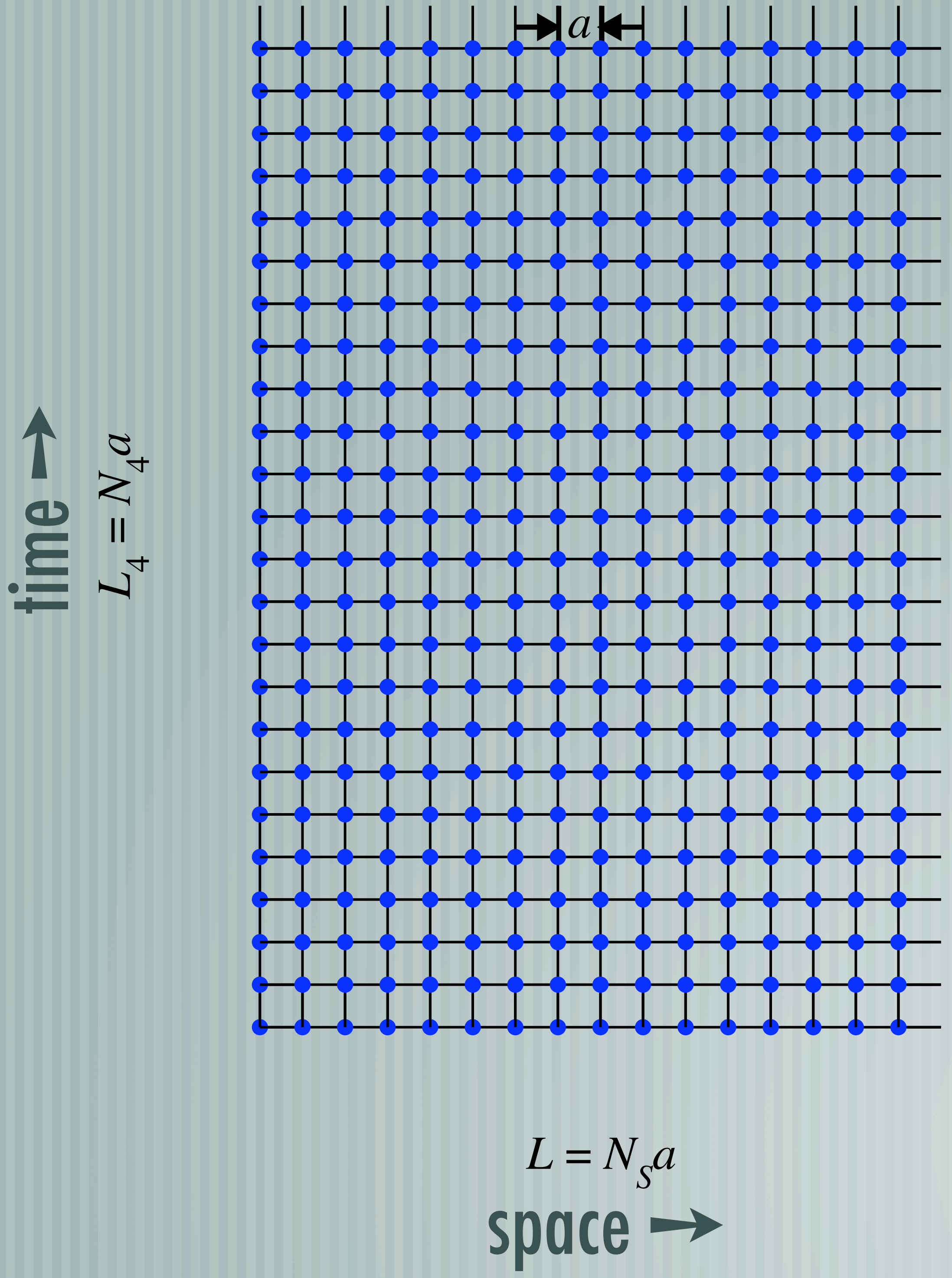


Lattice QCD

Lattice Gauge Theory

- Feynman functional-integral formulation of QFT:
  - everything is a (infinite-dimensional) integral.
- Field theory defined on a space-time lattice.
- Wilson (1974) showed how to put non-Abelian gauge symmetries into lattice field theory.
- A simple and compelling explanation of confinement.

Spacetime Lattice



- Spacing a gives UV cutoff
- Box-size L gives IR cutoff
- Euclidean metric $t = ix_4$ yields positive weight

Lattice QCD

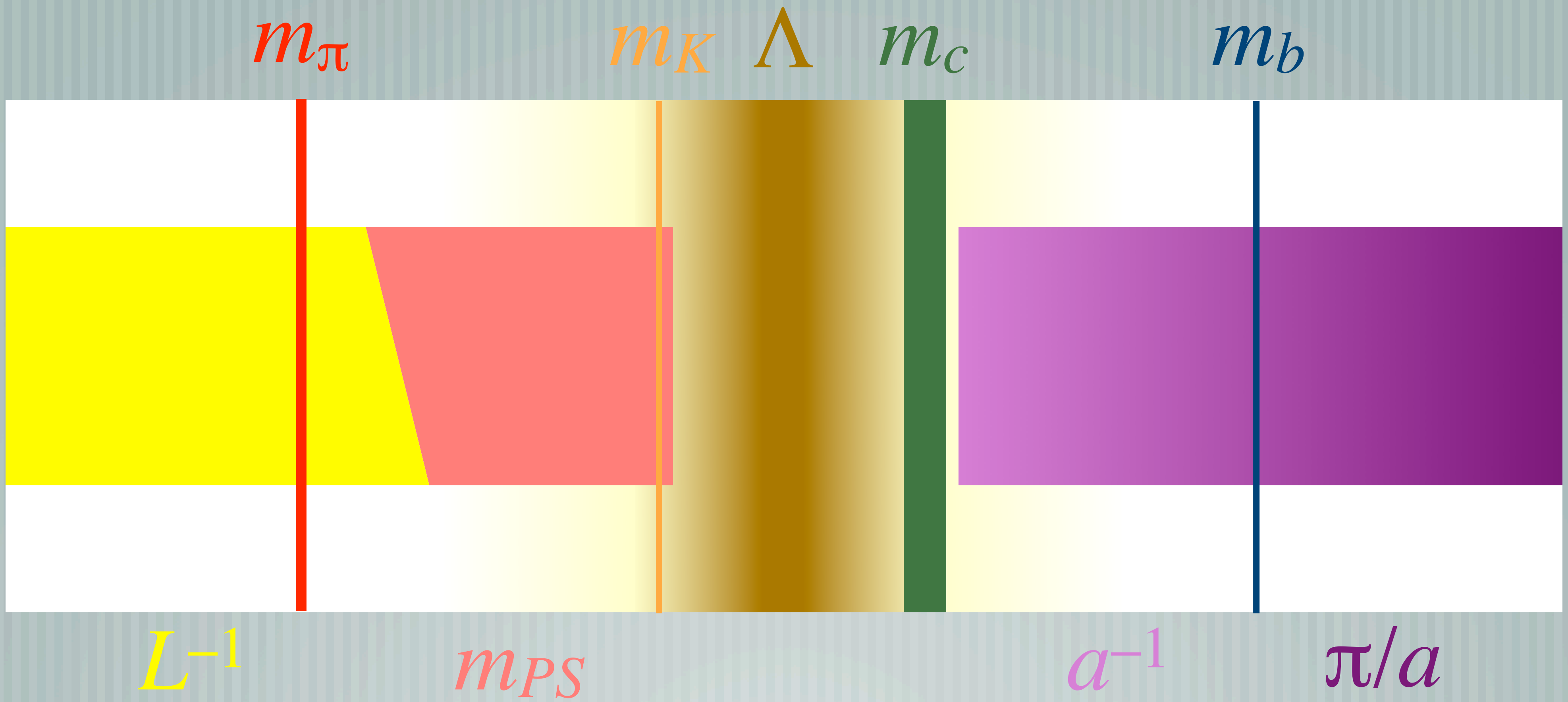
- Lattice gauge theory provides a non-perturbative definition
  - the Lagrangian of lattice QCD has $1 + n_f$ parameters.
- Lattice gauge theory + numerical simulation
  - compute the integrals numerically.
- With $a \neq 0$ and L, $L_4 < \infty$ the problem is finite.
- With positive weights, Monte Carlos methods work.

Many Scales in QCD

- Characteristic scale, Λ_{QCD}, around $m_\rho = 770$ MeV
  - coupling $\alpha_s(q) \sim 1$ for $q \sim 250$ MeV
  - chiral symmetry scale $m_K^2/m_s \approx 2500$ MeV
- Light quarks: $m_u, m_d \ll m_s \sim 80$ MeV $\ll \Lambda_{\mathrm{QCD}}$
- Heavy quarks: $m_b \gg m_c \approx 1400$ MeV $> \Lambda_{\mathrm{QCD}}$
- Top quark: $m_t \approx 175$ GeV, so decays before hadronizing.

Many Scales in Lattice QCD

QCD scales



MC scales

Many Scales in Physics

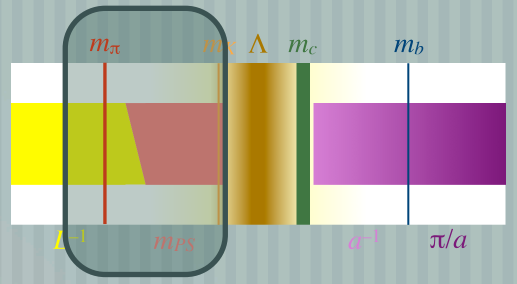
- Mercedes: So, some dude at Cornell won the Nobel Prize in physics this year [1982]. Do you know him?
- Andreas: Yes, I know Ken Wilson.
- Mercedes: What did he do?
- Andreas: He studied how to approach problems with more than one length scale. He said to study one scale at a time.
- Mercedes: What’s so clever about that?

Effective Field Theories

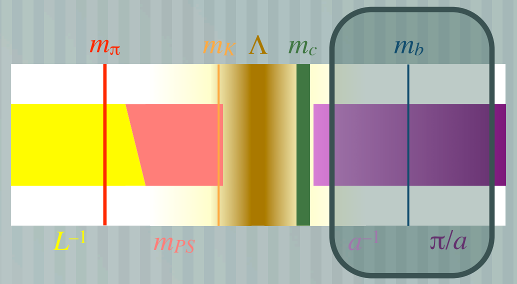
- A powerful framework for separating physics at different length scales.
- Effective Lagrangian
  - “short-distance” physics lumped into coefficients,
  - “long-distance” physics described by operators.
- Cascade of EFTs; matching calculations.

EFTs in Lattice QCD

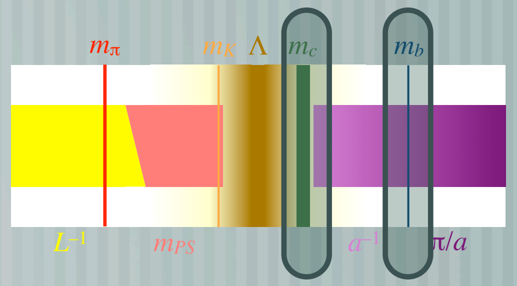
- Chiral perturbation theory for the pion cloud
  - to extrapolate in light quark mass.



- Symanzik theory of cutoff effects
  - for gluons and light quarks.



- Heavy-quark theories (HQET and NRQCD)
  - for cutoff effects of heavy quarks.



Lattice Fermions

- Naïve: 16 species per field, lately called "tastes".
- Wilson: 1 taste (flavor), but hard chiral symmetry breaking $\Rightarrow$ fine tuning $\Rightarrow m_q > 0.7 m_s$ [JLQCD, QCDSF, ...].
- Staggered: still 4 tastes per field, but remnant of chiral symmetry $\Rightarrow m_q > 0.15 m_s$ [MILC].
- Ginsparg-Wilson (domain wall or overlap): flavor simple, full chiral symmetry.

The Berlin Wall

$$\texttt{cost} \propto \left(\frac{m_V^2}{m_{PS}^2}\right)^3 L^{4+1}\, a^{-(4+3)}$$

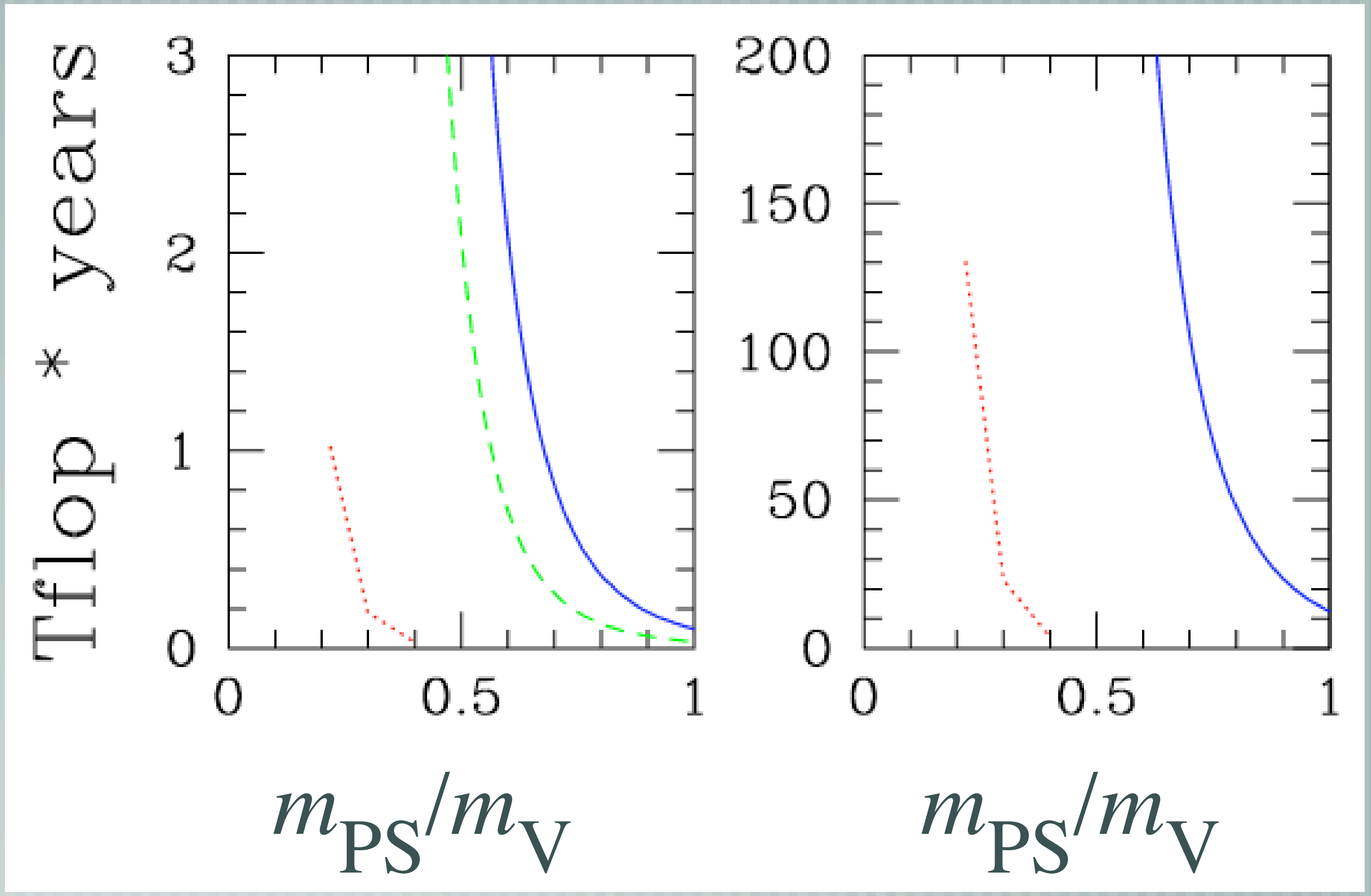
cost for Wilson

3 times faster

cost for staggered

Plot from Jansen, Ukawa & Gottlieb

hep-lat/0311039



a = 1/11 fm

measured in simulation

a = 1/22 fm

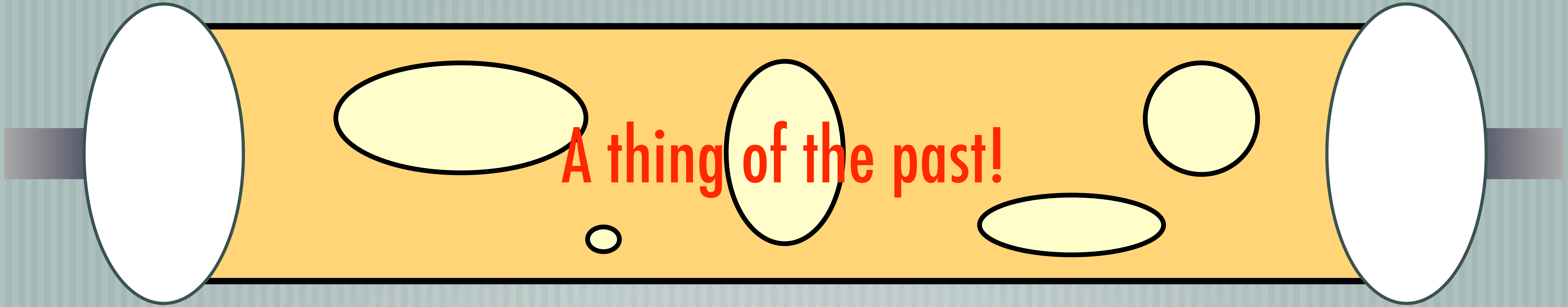
extrapolated

Chiral Extrapolation

- The slow-down at small quark mass has two important implications:
  - extrapolations in light quark masses are needed;
  - only staggered quarks are, so far, light enough to take chiral perturbation theory as a guide.
- Other methods catching up: 3-5 years behind.

Quenched Approximation

Full QCD has (expensive) quark loops.



- Replace $\det M$ with 1, and compensate by shifting bare gauge coupling and bare masses. “Dielectric”.
- Arguably OK if all light quarks had mass $m_q \sim \Lambda$.

Success (at last)

Staggered Quarks

- Staggered fermions have always been fast.
- Discretization effects $O(a^2)$, but “large”.
- Traced to “taste-changing” interactions.
- Systematically removed by Orginos, Sugar, & Toussaint:
- Remaining $O(a^2)$ removed by Lepage
  - the “asqtad action”: $O(\alpha_s a^2)$, $O(a^4)$ and “small”.

Gold-plated Quantities

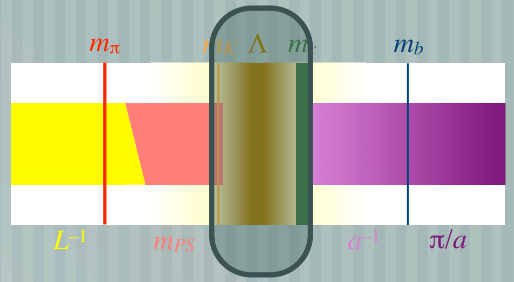
- Some quantities are under much better control:
  - 1 hadron in the initial state & 0 or 1 in the final state;
  - stable, or narrow and not too close to threshold.
- Chiral extrapolation must also be under control!
- Narrow D^*, ϕ, ... not gold-plated, but perhaps not bad.
- (almost) elastic ρ, Δ, $K \to \pi\pi$ much, much harder.

The MILC Ensembles

- MILC Collaboration = dozen or so physicists at Arizona, UCSB, APS, Indiana, Pacific, Utah, Washington U. (St. Louis)
- Improved staggered quarks (asqtad action)
- 2 + 1 flavors of light quarks in sea
- Lattice spacings $a = 1/8,\ 1/11\ \mathrm{fm.}$

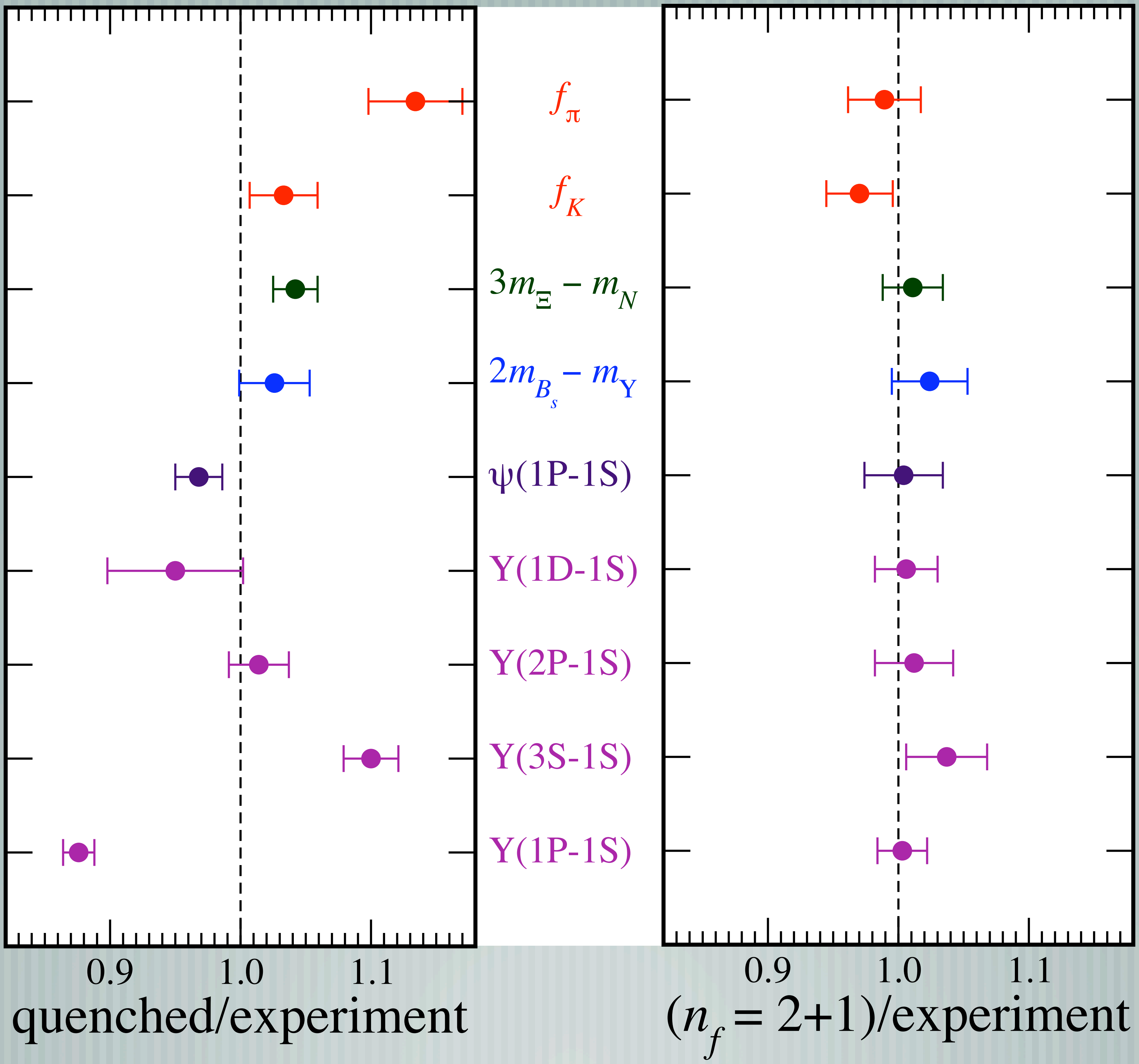
- Many (valence and sea) m_q down to $0.15m_s$.
- Several hundred lattice gauge fields per ensemble
  - sub-% statistical errors (importance sampling).
- Freely available over the internet.

- Several groups started looking at light hadrons (MILC), hadrons with bottom quarks (HPQCD), & hadrons with charmed quarks (Fermilab).
- All of the QCD scale was being probed.



- A consistent picture emerged: after tuning $1 + n_f$ parameters, we checked 9 other mass splittings and decay constants.

Davies et al., hep-lat/0304004



Update: Ω^- works too!

The Dark Side

- Because staggered quarks come in four tastes, we have used $[\det_4 M]^{1/4}$ for $\det_1(\not{D} + m)$.
- But $\det_4 M^{1/4}$ looks non-local and, hence, terrifying.
- Several theoretical and numerical studies are suggestive that the "¼-root trick" is acceptable.
- Nevertheless, "not proven:" not proven right; not proven wrong either.

Summary So Far

- Lattice QCD with improved staggered quarks agrees with Nature for 5+9 gold-plated quantities.
- Only improved staggered fermions have achieved the following:
  - 2+1 flavors of sea quark
  - quarks light enough for chiral perturbation theory
- Very promising for flavor physics and all QCD.

Examples

- Marciano suggests taking $f_\pi/f_K = 1.210(4)(13)(1)$ [MILC] to get the Cabibbo angle $\tan\theta_{12} = |V_{us}|/|V_{ud}|$
- Quark masses [MILC/HPQCD]
  - strange $m_s(2\ \mathrm{GeV}) = 76(0)(3)(0)(7)\ \mathrm{MeV}$
  - $2m_s/(m_u + m_d) = 27.4(4)$; $m_u/m_d = 0.43(8)$
- Strong coupling [HPQCD] $\alpha^{(5)}_{\overline{\mathrm{MS}}}(M_Z) = 0.1177(13)$

Predictions

Predictive Lattice QCD

- Any numerical simulation is a messy enterprise.
- An end-to-end test is a fair demand.
- Compute something before it’s been measured.
- Success (?!) in a strongly-coupled field theory.
- Use calculations of unmeasurable quantities to learn more about deep questions about quarks.

- Fortunately, we are in a position to make some:
  - semi-leptonic form factor of the D meson, $f_+(q^2)$
    - normalization,
    - shape;
  - leptonic decay of the D meson, f_D;
  - mass of the B_c meson, m_{Bc}.
- All being measured on the same time scale, or a little later!

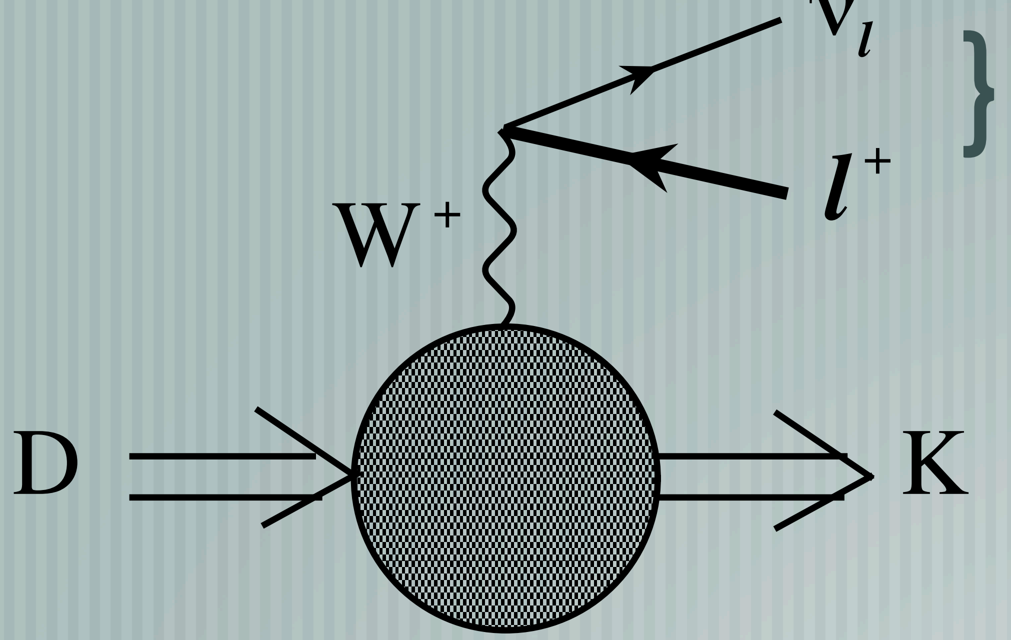
Tests several ingredients

calculation	light sea	light valence	heavy
semileptonic f_+	★★	★★	★★
leptonic f_D	★★	★★★	★★
B_c mass	★★	—	★★★

Let's see how we are doing!

$f_+^{D\to\pi}(q^2)$ & $f_+^{D\to K}(q^2)$

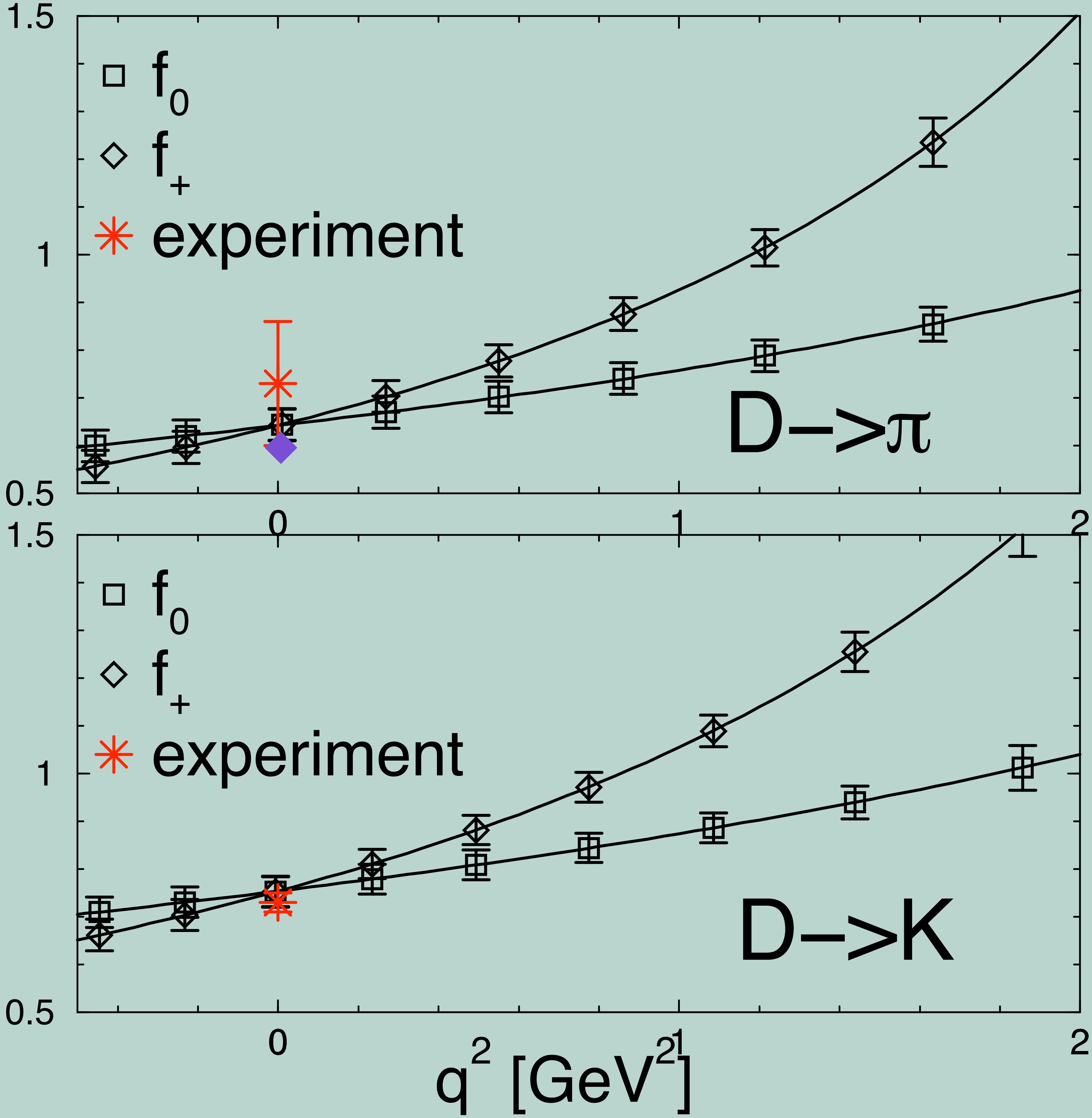
Semileptonic Decay



$$q^2 = m_D^2 + m_K^2 - 2m_D E$$

$$\frac{d\Gamma}{dE} = \frac{G_\mu^2 m_D}{12\pi^3}|V_{cs}|^2 p^3 |f_+(E)|^2$$

$$\langle K(p_K)|V^\mu|D(p_D)\rangle = f_+(E)\left[p_D + p_K - \frac{m_D^2 - m_K^2}{q^2}q\right]^\mu + f_0(E)\frac{m_D^2 - m_K^2}{q^2}q^\mu$$


1.5
1
0.5
f_0
f_+
experiment
D->π
0
1
2
1.5
1
0.5
f_0
f_+
experiment
D->K
0
1
2
q² [GeV²]

hep-ph/0408306

dominant error:
heavy quark
discretization

- $D \to Kl\nu$:

  $$f_+^{D\to K}(0) = 0.73(3)(7)$$

  $$f_+^{D\to K}(0) = 0.78(5)$$ [BES, hep-ex/0406028]

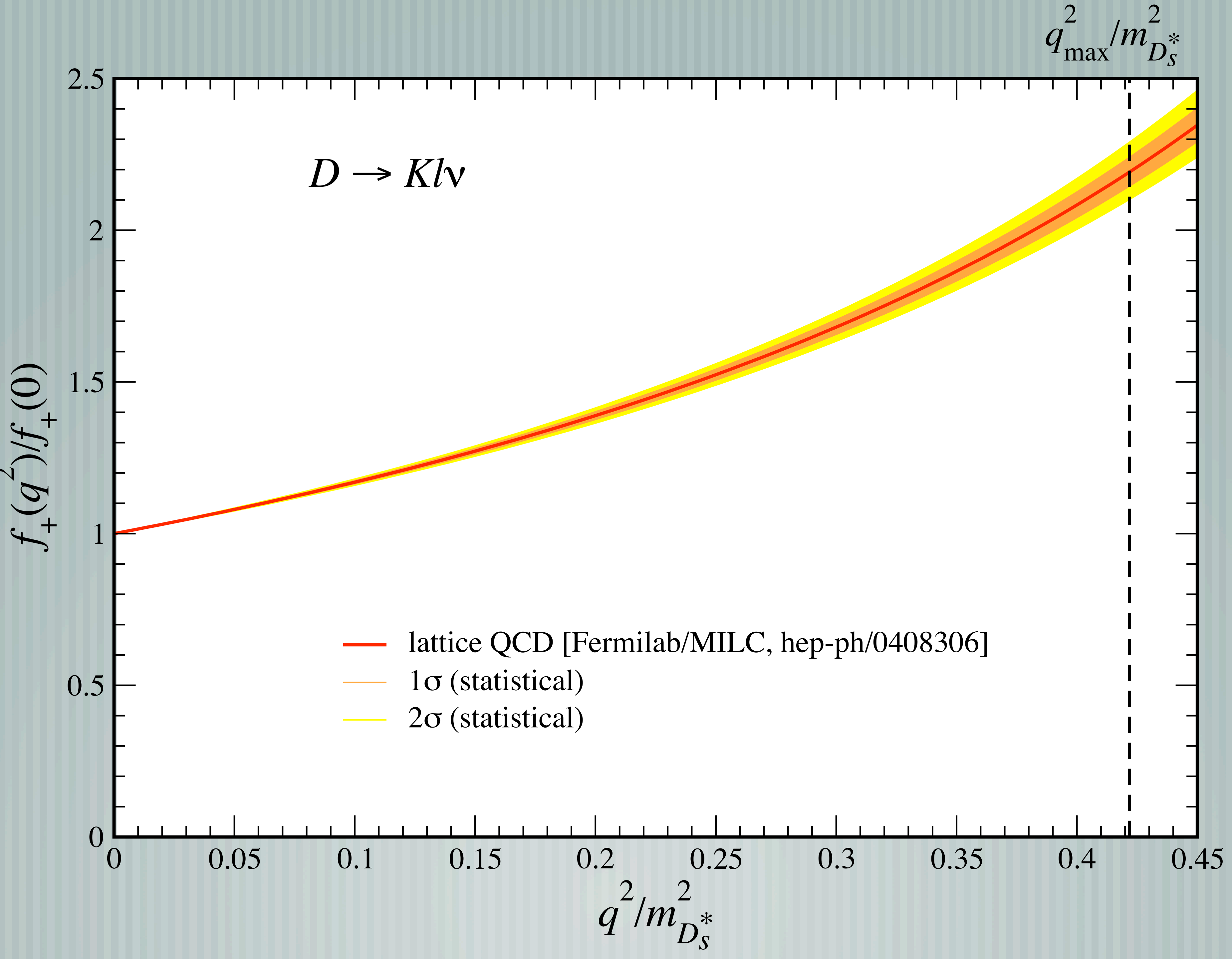
- $D \to \pi l\nu$:

  $$f_+^{D\to \pi}(0) = 0.64(3)(6)$$

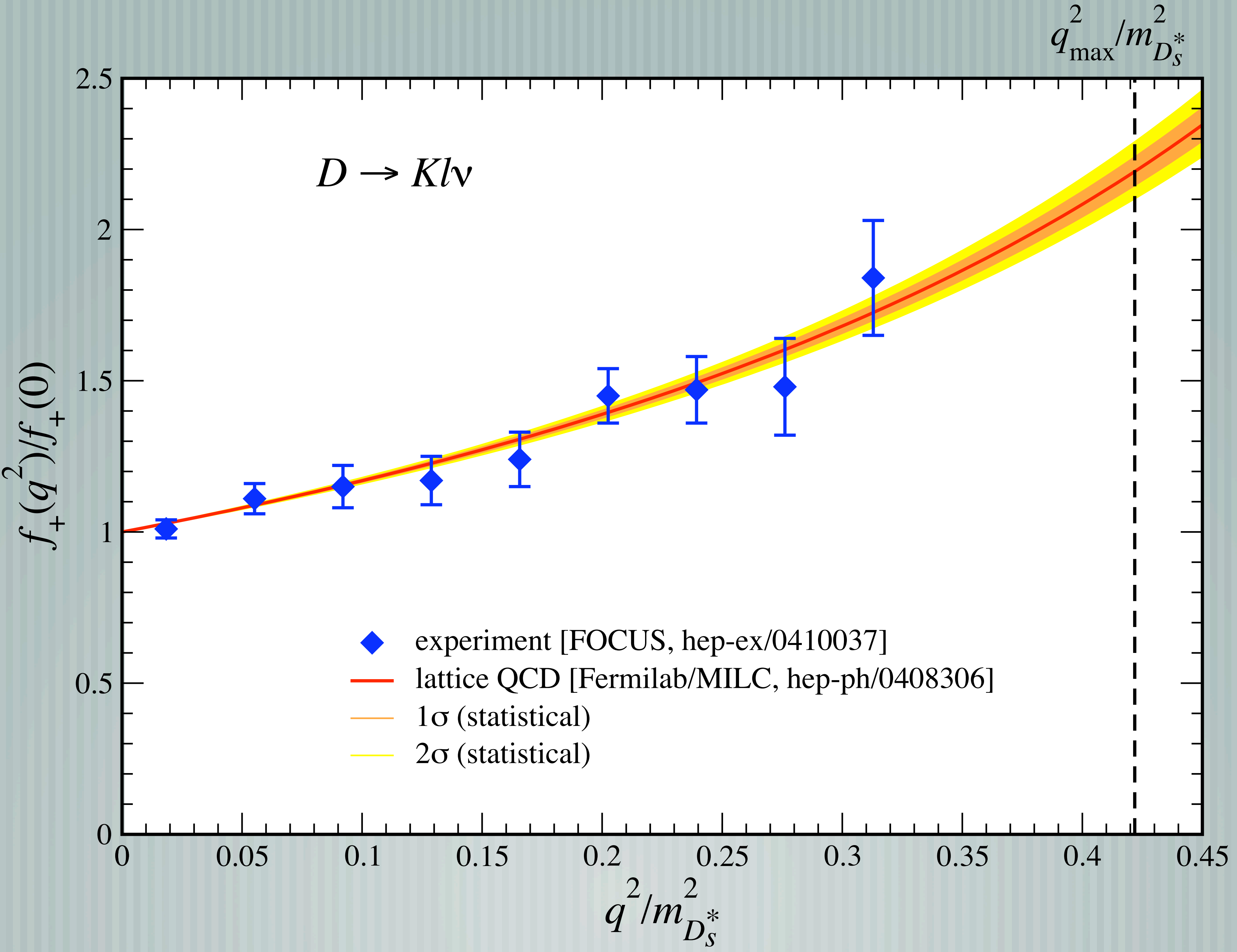
  $$f_+^{D\to \pi}(0) = 0.87(3)(9) f_+^{D\to K}$$

  $$f_+^{D\to \pi}(0) = 0.86(9) f_+^{D\to K}$$ [CLEO, hep-ex/0407035]

$D \to Kl\nu$ vs. q^2



$D \to K l \nu$ vs. q^2



Summary of Form Factors

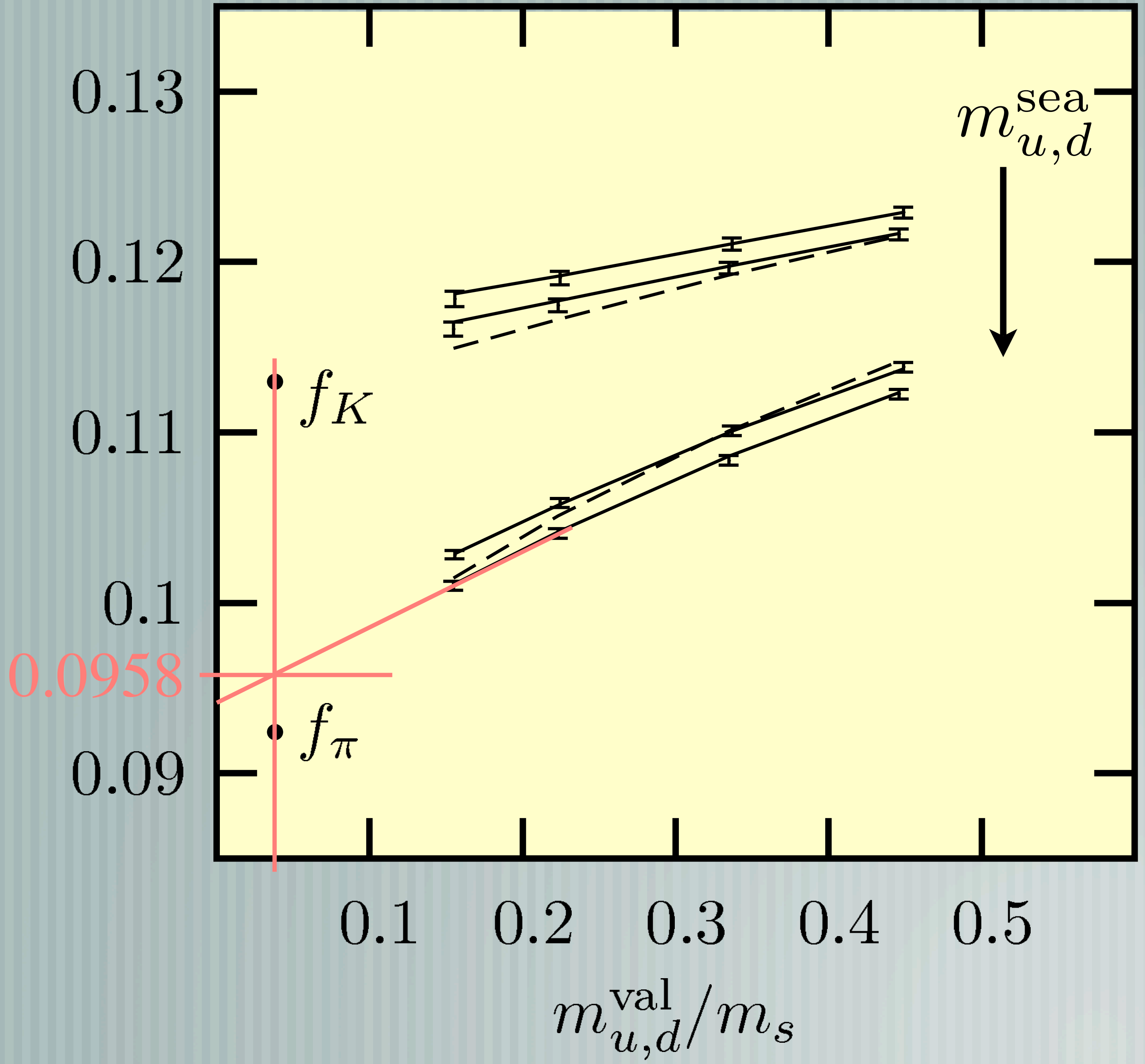
- BES and CLEO-III have confirmed the normalization, on the same time scale as our calculations.
- FOCUS confirmed the shape, after we were finished.
- CLEO-*c* will improve the measurements.
- Lattice can systematically improve: few % foreseeable.
- Prototype for $B \to \pi l \nu$, which yields $|V_{ub}|$.

f_{Ds} & f_D

f_{Ds} & f_D

- Meson decay constants parametrize $D \to l\nu$, etc.
- Experiments measure $|V_{cd}|f_D$ and $|V_{cs}|f_{Ds}$ ...
  - ... so take $|V_{cd}|$ and $|V_{cs}|$ from CKM unitarity.
- CLEO-c is measuring them.
- A test of chiral perturbation theory for staggered quarks.
- Prototype for f_B: no experiment will measure $|V_{ub}|f_B$.

Chiral Extrapolation



Dots are PDG.

Error bars are latQCD.

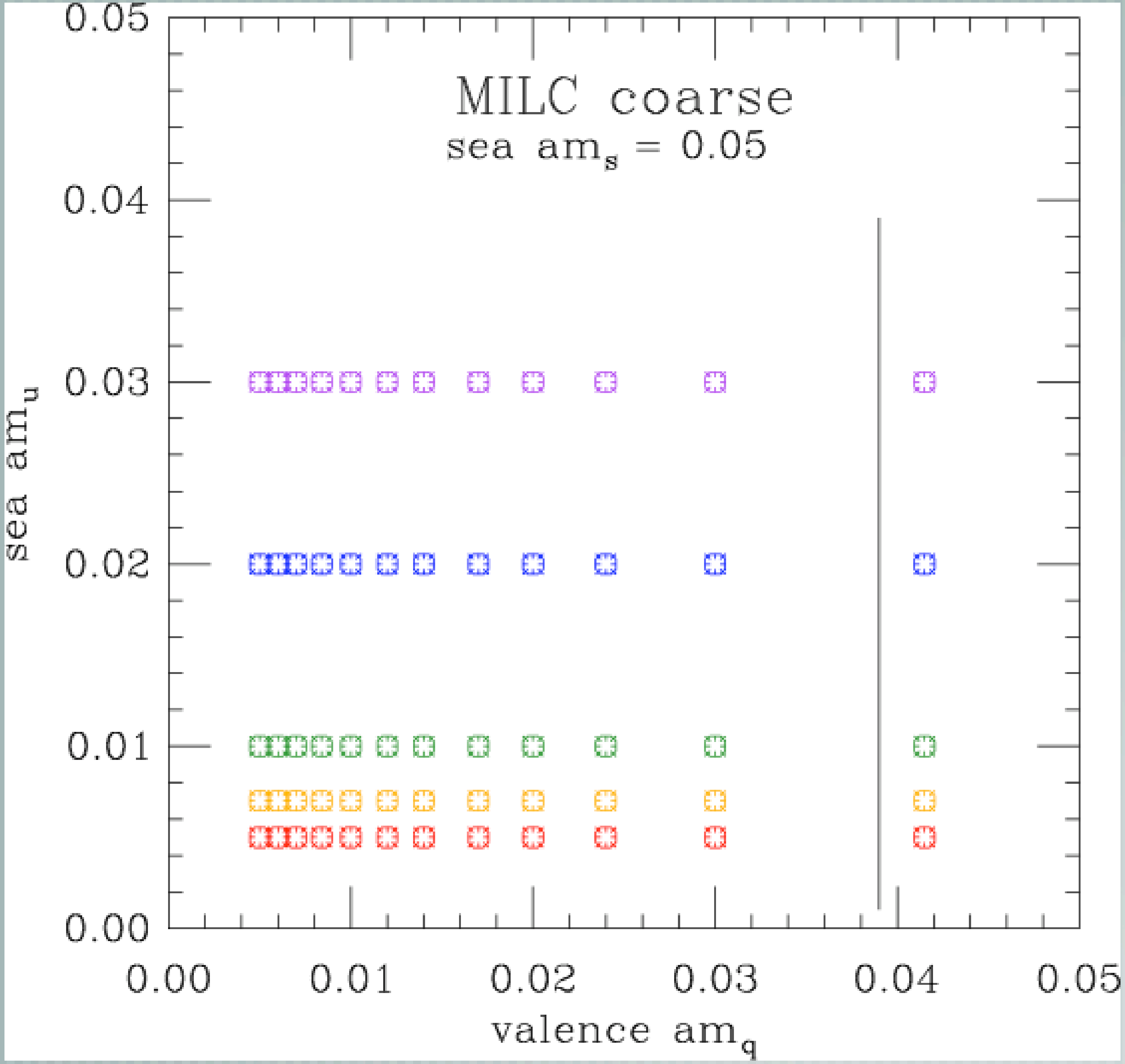
Linear extrap (demo).

Fancier versions of χPT get closer & improve CL.

Analysis Steps

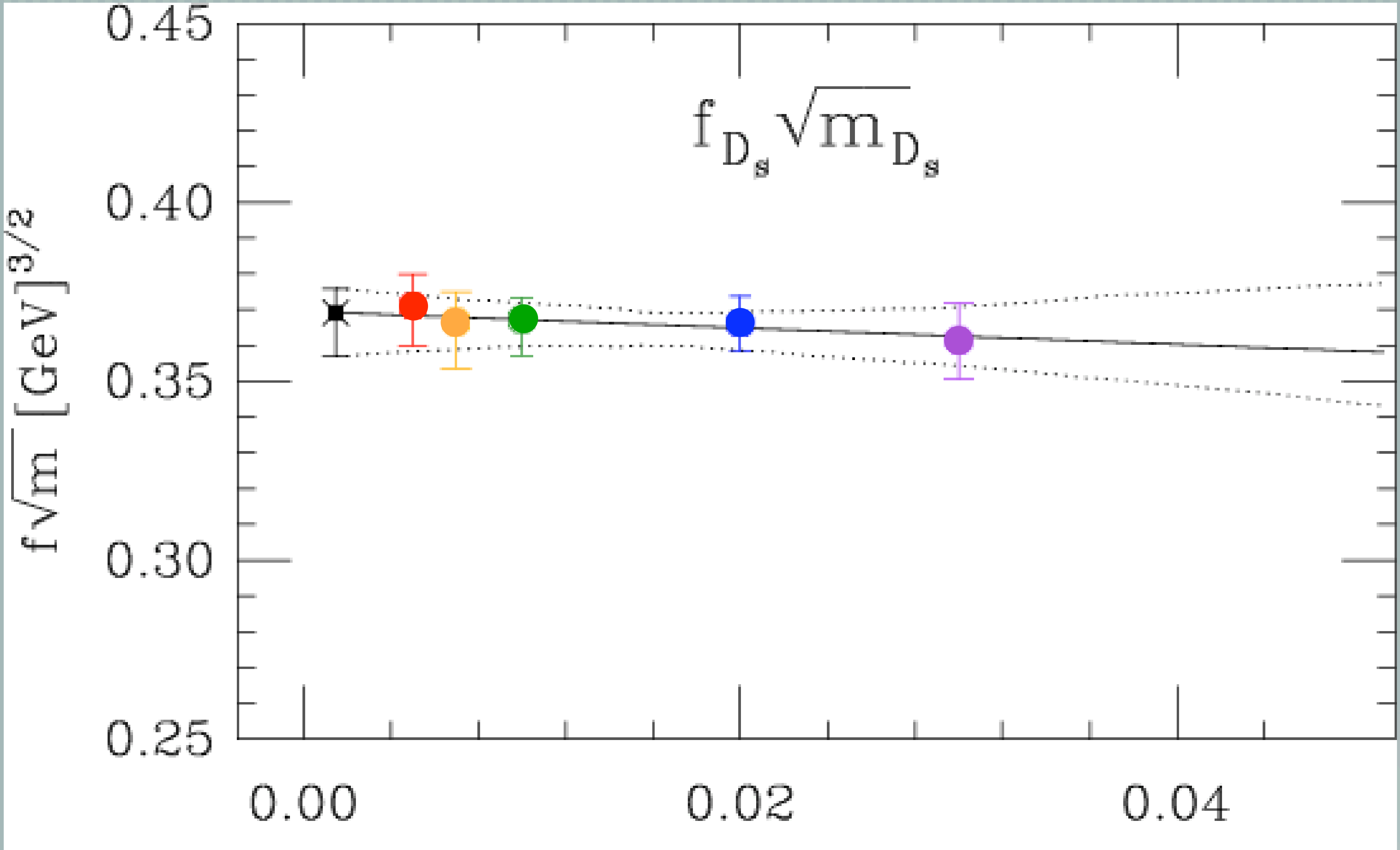
- Consider two quantities with different dominant uncertainties:
  - $\phi_s = f_{D_s}\sqrt{m_{D_s}}$ not sensitive to light quarks
  - $R_{d/s} = \phi_d/\phi_s$ most uncertainties cancel,
    (not most of the uncertainty cancels).

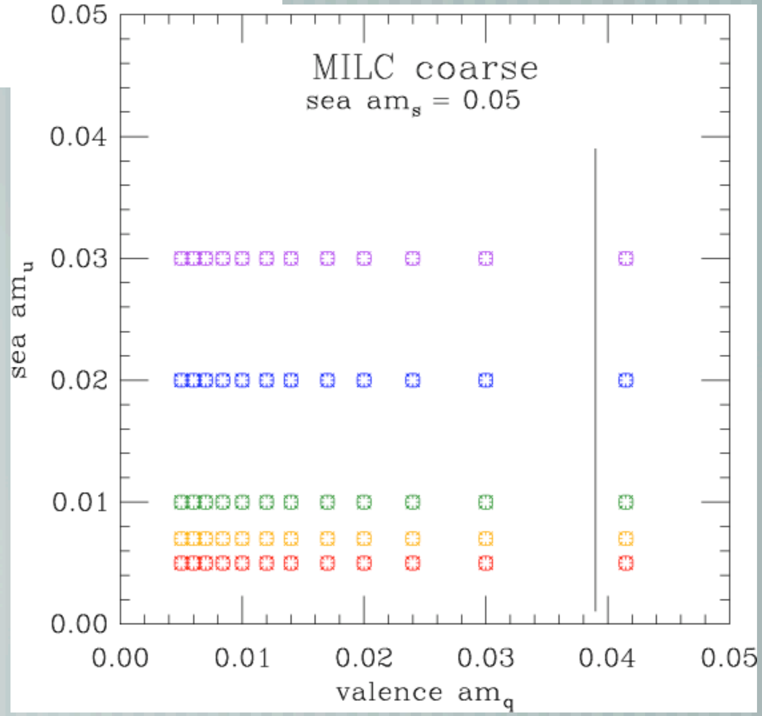
Chiral Extrapolation f_{Ds}



Interpolate in valence m_q to get down to real m_s.

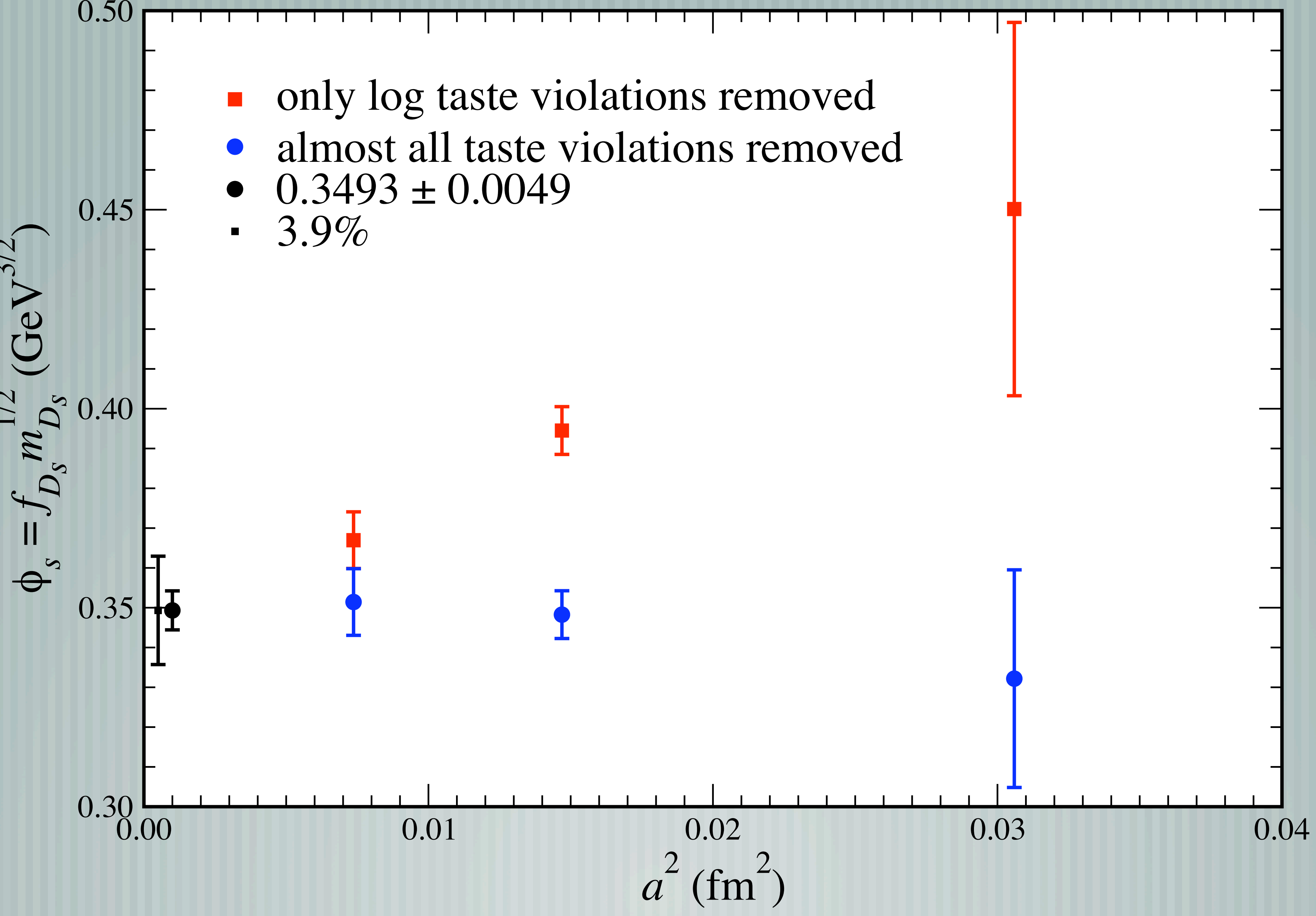
Extrapolate in sea m_u to get down to real m_l.



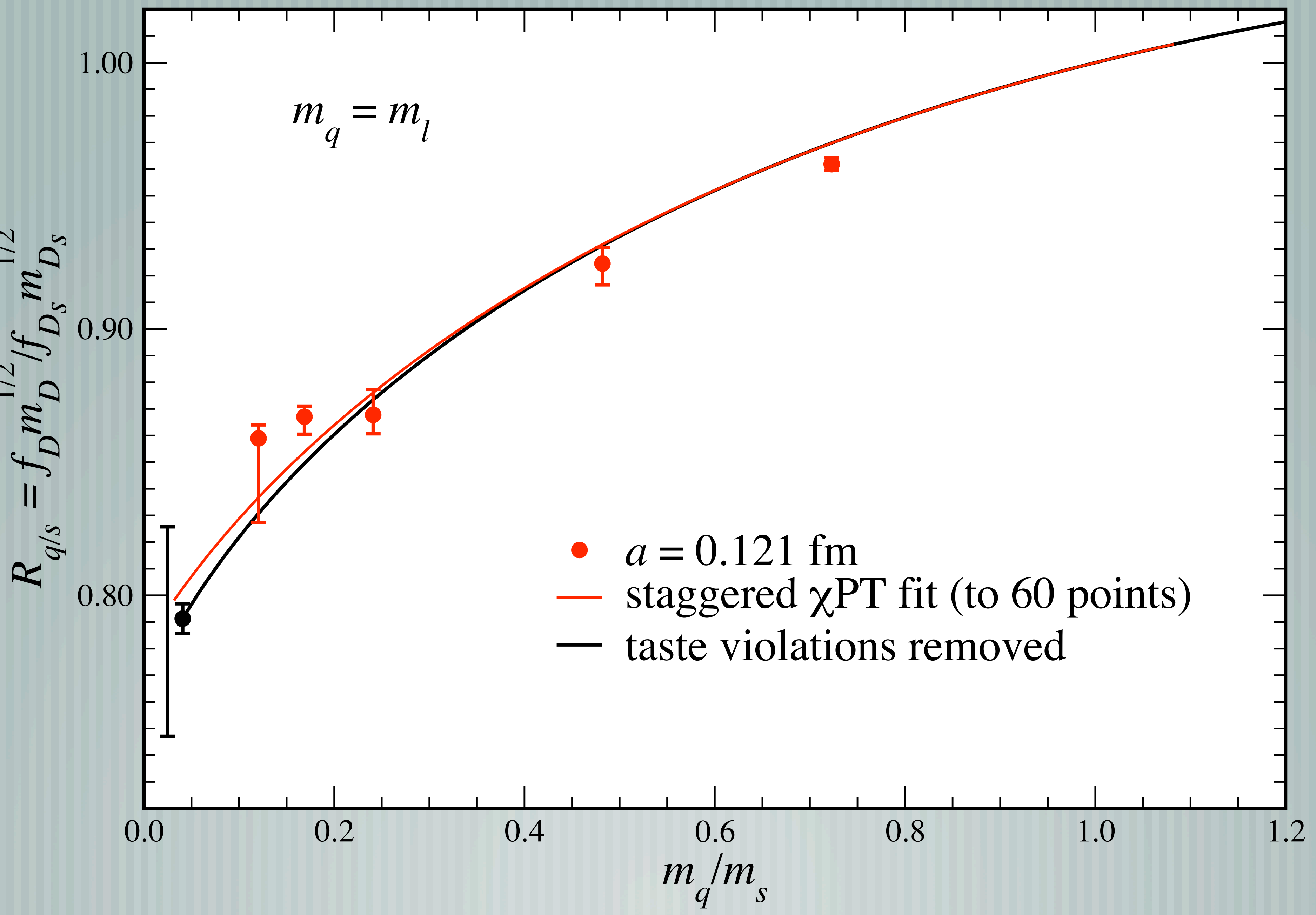


A separate linear fit,
shown for illustration.

Lattice Spacing Dependence



Chiral Extrapolation f_D



Final Results

- C. Aubin et al., hep-lat/0506030 (PRL)

$$\begin{aligned} R_{d/s} &= 0.786(04)(05)(04)(42) \\ \phi_s &= 0.349(05)(10)(15)(14)\ \mathrm{GeV}^{3/2} \end{aligned}$$

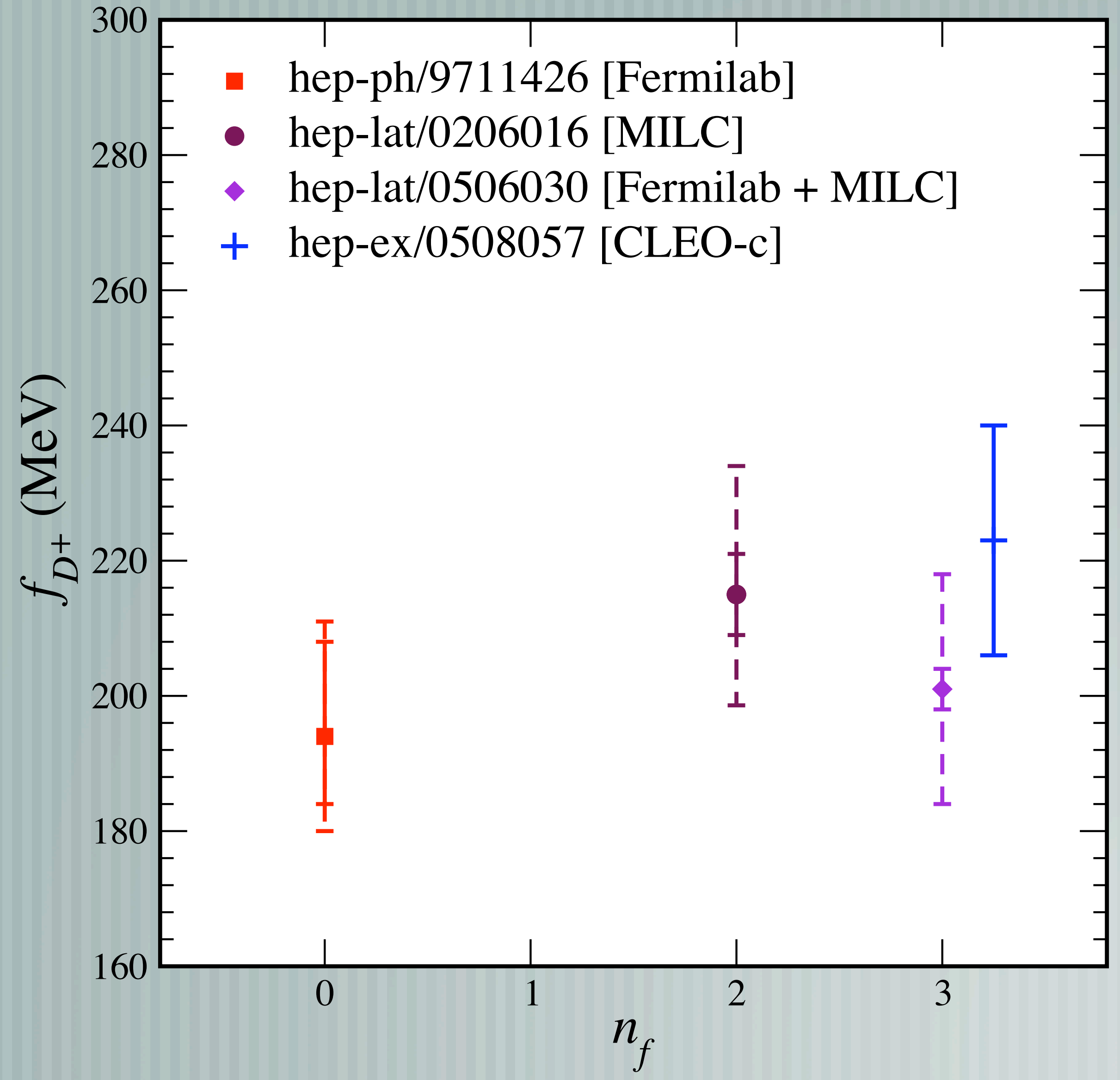
$$f_{D_s} = 249 \pm 3 \pm 7 \pm 11 \pm 10\ \mathrm{MeV}$$

$$f_{D^+} = 201 \pm 3 \pm 6 \pm 9 \pm 13\ \mathrm{MeV}.$$

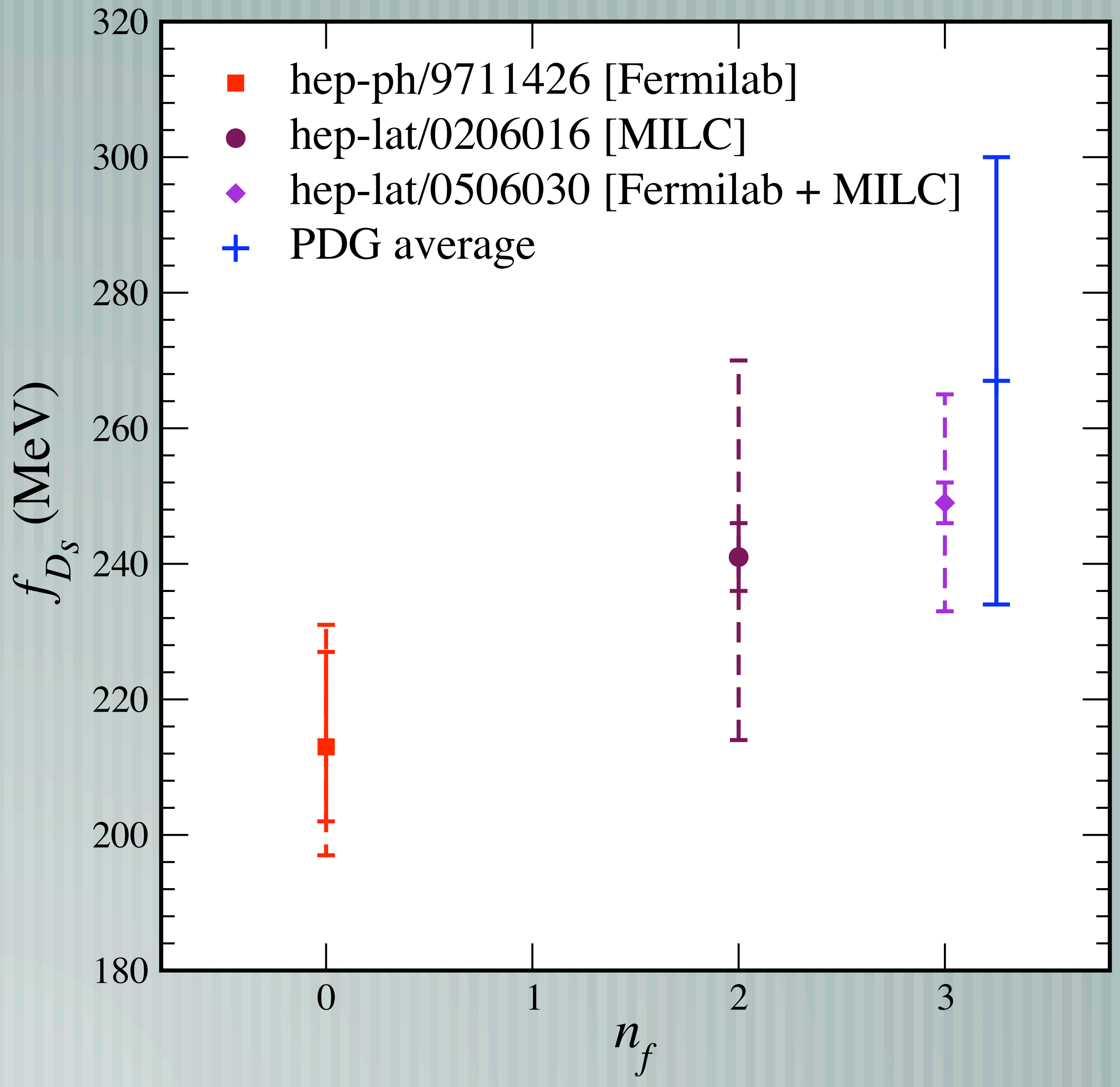
$$f_{D^+} = 223 \pm 17 \pm 3\ \mathrm{MeV}$$

CLEO-c, hep-ex/0508057

Comparison



■ hep-ph/9711426 [Fermilab]
● hep-lat/0206016 [MILC]
◆ hep-lat/0506030 [Fermilab + MILC]
+ hep-ex/0508057 [CLEO-c]
f_{D^+} (MeV)
300
280
260
240
220
200
180
160
0
1
2
3
n_f



■ hep-ph/9711426 [Fermilab]
● hep-lat/0206016 [MILC]
◆ hep-lat/0506030 [Fermilab + MILC]
+ PDG average
f_{D_s} (MeV)
320
300
280
260
240
220
200
180
0
1
2
3
n_f

B_c

B_c

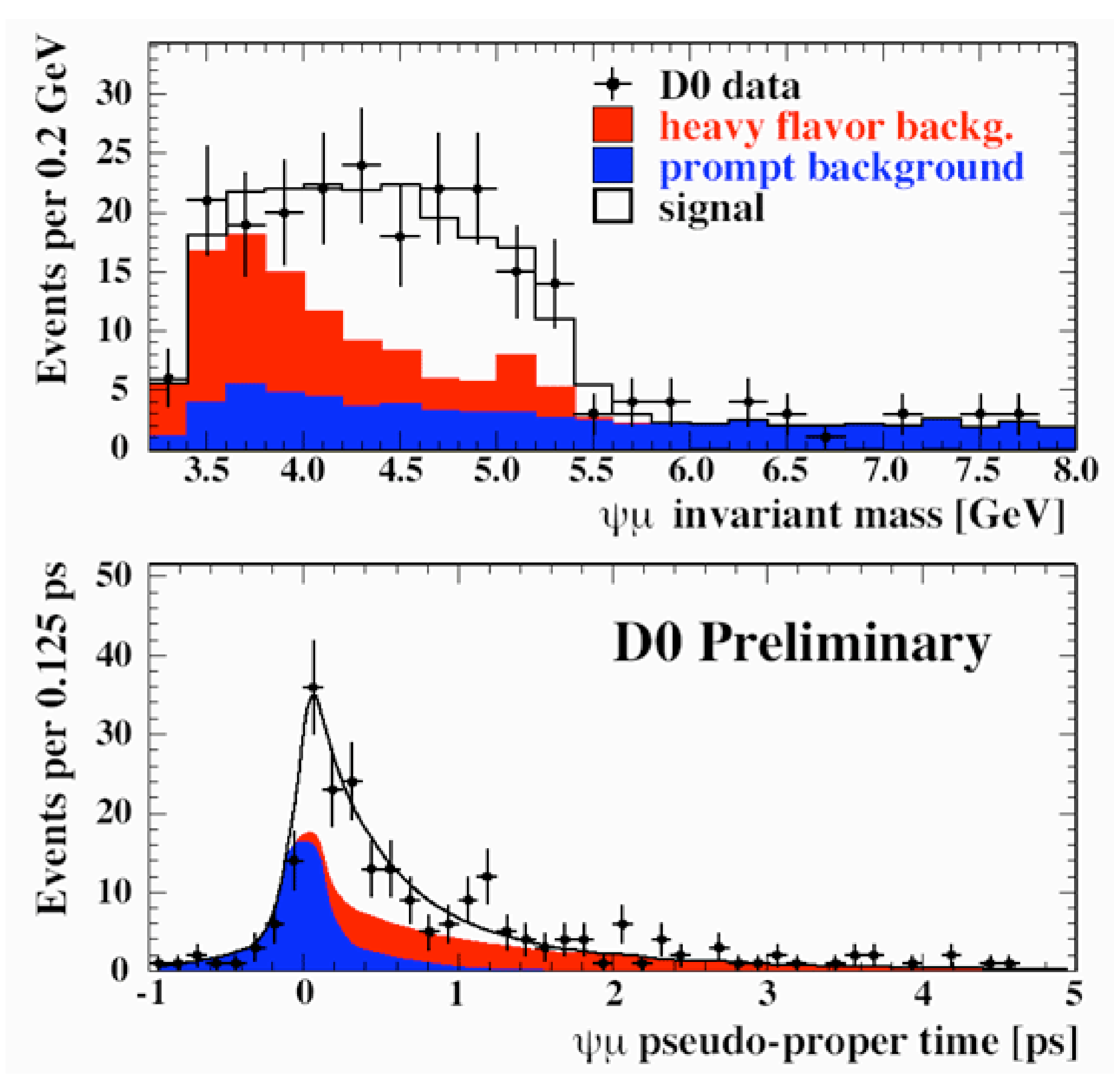
- Meson composed of a beautiful anti-quark and a charmed quark.
- Unusual beast
  - contrast with B_s & D_s, ψ & Υ: $v_c = 0.7$.
  - no annihilation to gluons

Fermilab *Today*

Thursday & Friday, December 2 & 3, 2004

Fermilab Result of the Week

DØ



Fermilab Result of the Week

CDF

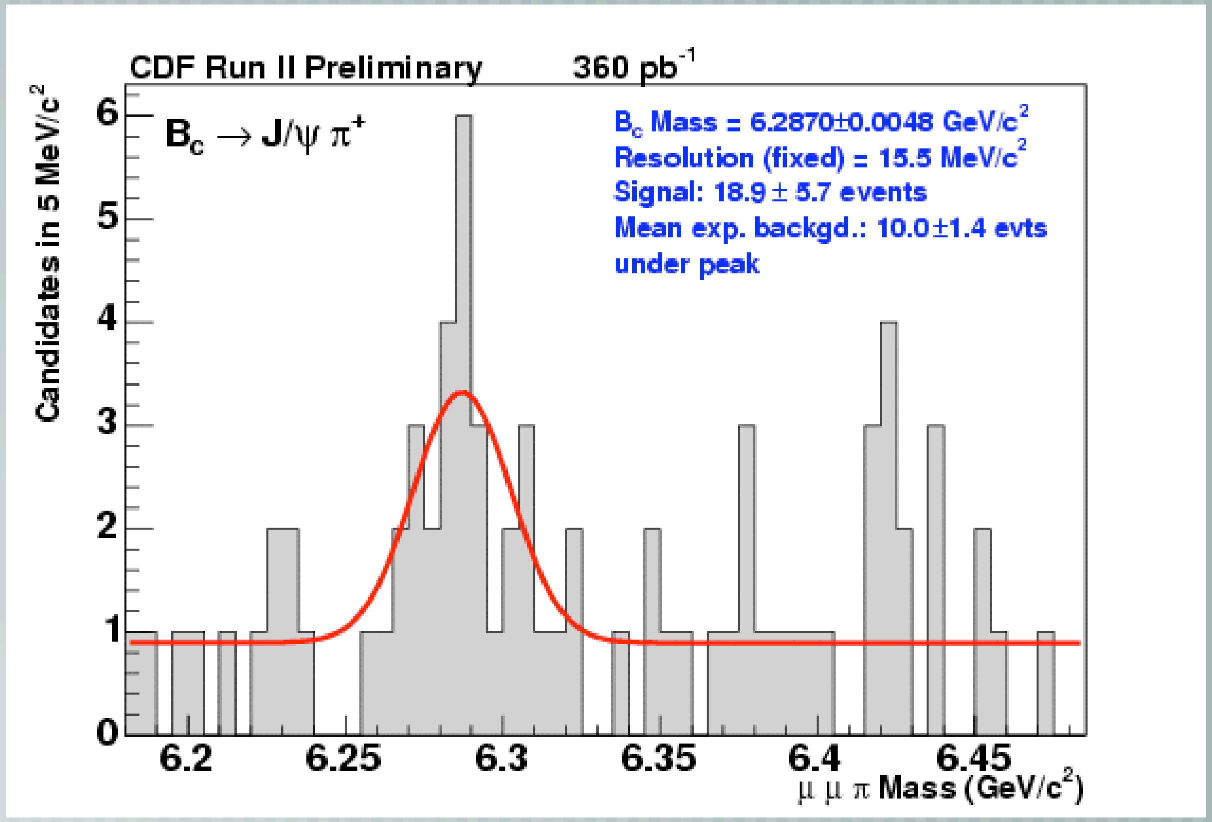
4:00 p.m. One West

Joint Experimental Theoretical Physics Seminar

Saverio D'Auria, University of Glasgow

B_c: Fully Reconstructed Decays and

Mass Measurement at CDF



QCD Theory & B_c

- Three main tools
  - potential models
  - potential NRQCD
  - lattice QCD
- All treat both quarks as non-relativistic
  - charmed quark is pushing it, $v_c^2 = 0.5$.

Essentials

- Prediction: α_s, m_b, m_c taken from bottomonium and charmonium spectrum
- Use latNRQCD for b and Fermilab method for c.
- We calculate two mass splittings
  - $\Delta_{\psi\Upsilon} = m_{B_c} - \frac{1}{2}(\bar{m}_\psi + m_\Upsilon)$ quarkonium baseline
  - $\Delta_{D_sB_s} = m_{B_c} - \frac{1}{2}(\bar{m}_{D_s} + \bar{m}_{B_s})$ heavy-light baseline

Error Analysis

- Everything is gold-plated, in the sense that the mesons are all stable, and far from threshold.
- Statistical error is straightforward & small.
- Uncertainty from a^{-1}, m_b, m_c easy to propagate: latter two are ±10, ±5 MeV.
- Main problem is to estimate the discretization effect for the heavy quarks.

Discretization Effects

(short distance mismatch) • (matrix element)

- Use calculations of tree-level mismatches
- Wave hands for one-loop mismatches
- Estimate matrix elements in potential models
- Check framework with other calculations

Results

- Splittings:

$$\begin{aligned} \Delta_{\psi\Upsilon} &= 39.8 \pm 3.8 \pm 11.2^{+18}_{-\ 0}\ \mathrm{MeV}, \\ \Delta_{D_s B_s} &= -\left[1238 \pm 30 \pm 11^{+\ 0}_{-37}\right]\ \mathrm{MeV}, \end{aligned}$$

- Meson mass:

$$\begin{aligned} m_{B_c} &= 6304 \pm\ \ 4 \pm 11^{+18}_{-\ 0}\ \mathrm{MeV}, \\ m_{B_c} &= 6243 \pm 30 \pm 11^{+37}_{-\ 0}\ \mathrm{MeV}, \end{aligned}$$

- More checks on quarkonium baseline, so it is our main result.

Comparisons

$$m_{B_c}^{n_f=0} = 6386 \pm 9 \pm 15 \pm 98 \text{ MeV}$$

[Phys. Lett. B 453, 289 (1999)]

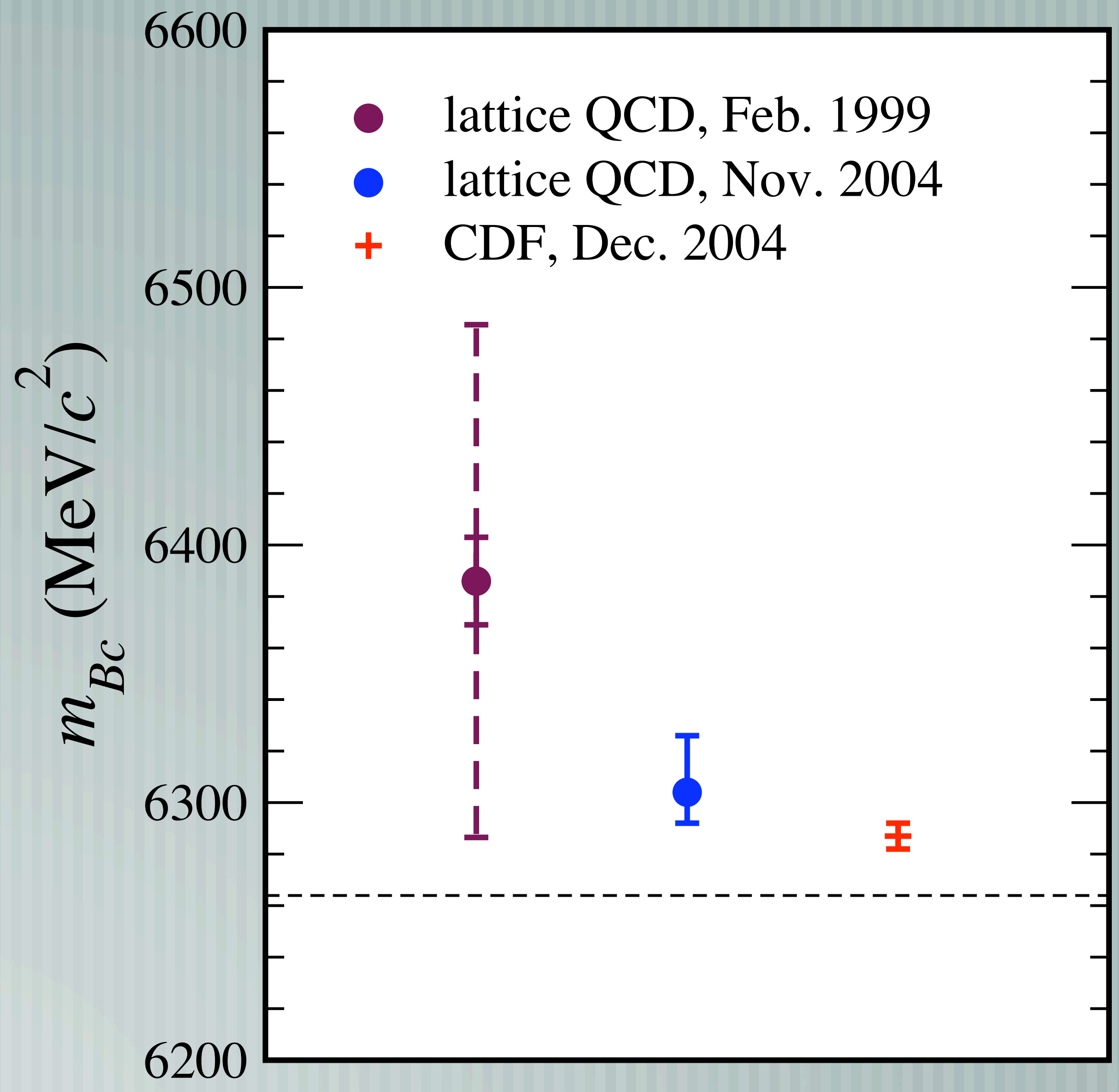
$$m_{B_c}^{2+1} = 6304 \pm 4 \pm 11^{+18}_{-0} \text{ MeV}$$

[`hep-lat/0411027` → PRL]

$$m_{B_c}^{\text{expt}} = 6287 \pm 5 \text{ MeV}$$

[CDF, W&C seminar, 12/3/2004]

hep-ex/0505076

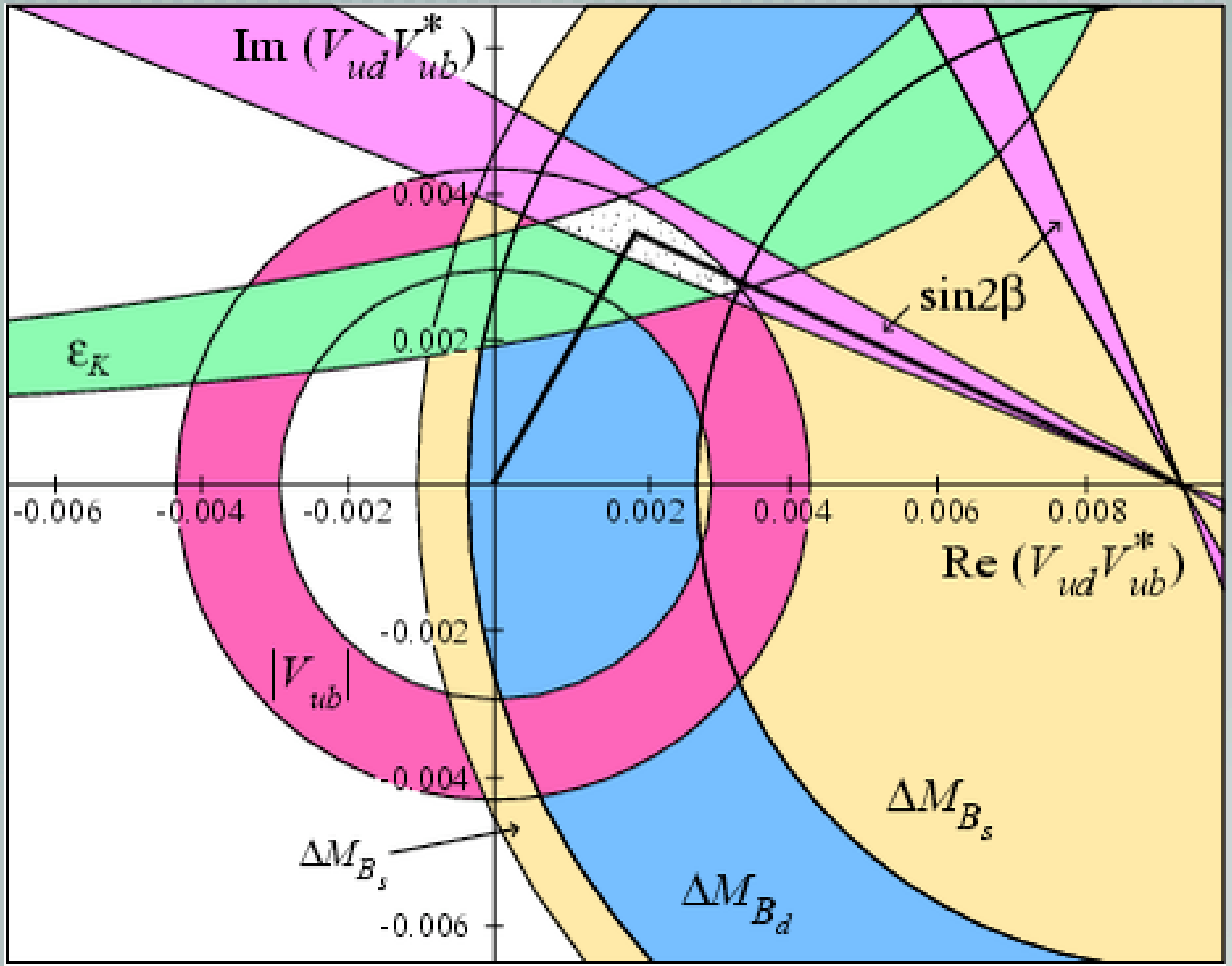


Outlook

Non-Perturbative QCD

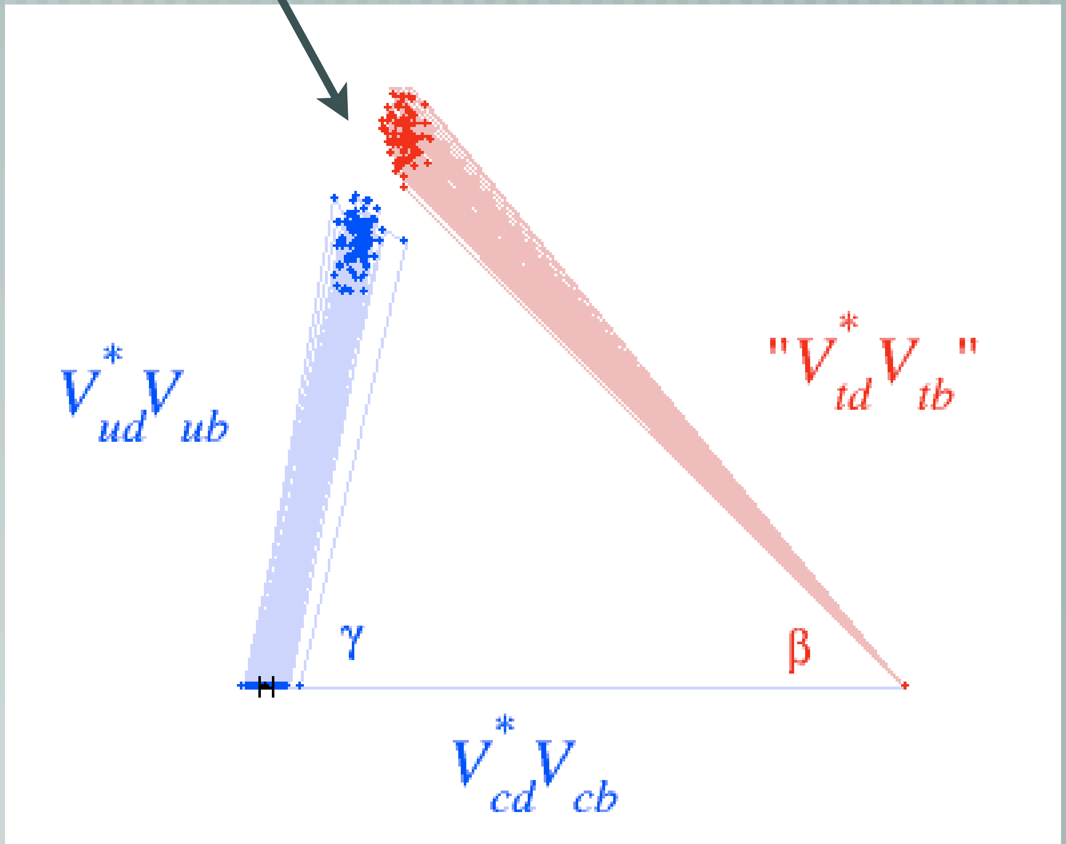
- The “end of the beginning” of non-perturbative QCD
  - even if staggered quarks prove not to be the last word, other methods are only 3-5 years behind.
- This advance opens the way to applications in flavor physics, RHIC and, of course, the LHC
  - QCD calculations of moments of parton densities;
  - new strong dynamics breaking $SU_L(2) \times U_Y(1)$.

MATRIX RELOADED



Mind the gap!

It's new physics!



Thanks

- MILC Collaboration
- Junior collaborators Masataka Okamoto, Ian Allison, Matthew Nobes, Christopher Aubin, ...
- Don Holmgren and Amitoj Singh