Lattice QCD Overview:
Understanding Uncertainty Budgets

(Estimation, Cogitation, Remonstration)

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Lattice QCD Meets Experiment: ⟨Lattice||Experiment⟩

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Kinds of Uncertainty

- Quantitative:
  - based on “theorems” and derived from (numerical) data;
- Semi-quantitative:
  - based on “theorems” but insufficient data to make robust estimates;
- Non-quantitative:
  - error exists but estimation is mostly subjective (or, hence, omitted);
- Sociological.

Sociology

- "Do you understand their error estimates? I don't."
  - could say this after detailed study of the calculation in question;
  - could say this just because you don't like the authors.
- Anecdote 1: Lepton-Photon Symposium, sometime in the last century.
- Anecdote 2: ILC-LHC apprehension vs. OPAL-D0 reality.
- My preferred criticism: "the calculation suffers from an uncertainty that is omitted from (underestimated in) the error budget."

Non-quantitative: Quenching Some or All Quarks

The Trouble with Determinants

- Early lattice-QCD calculations were carried out in the quenched approximation. What is it?

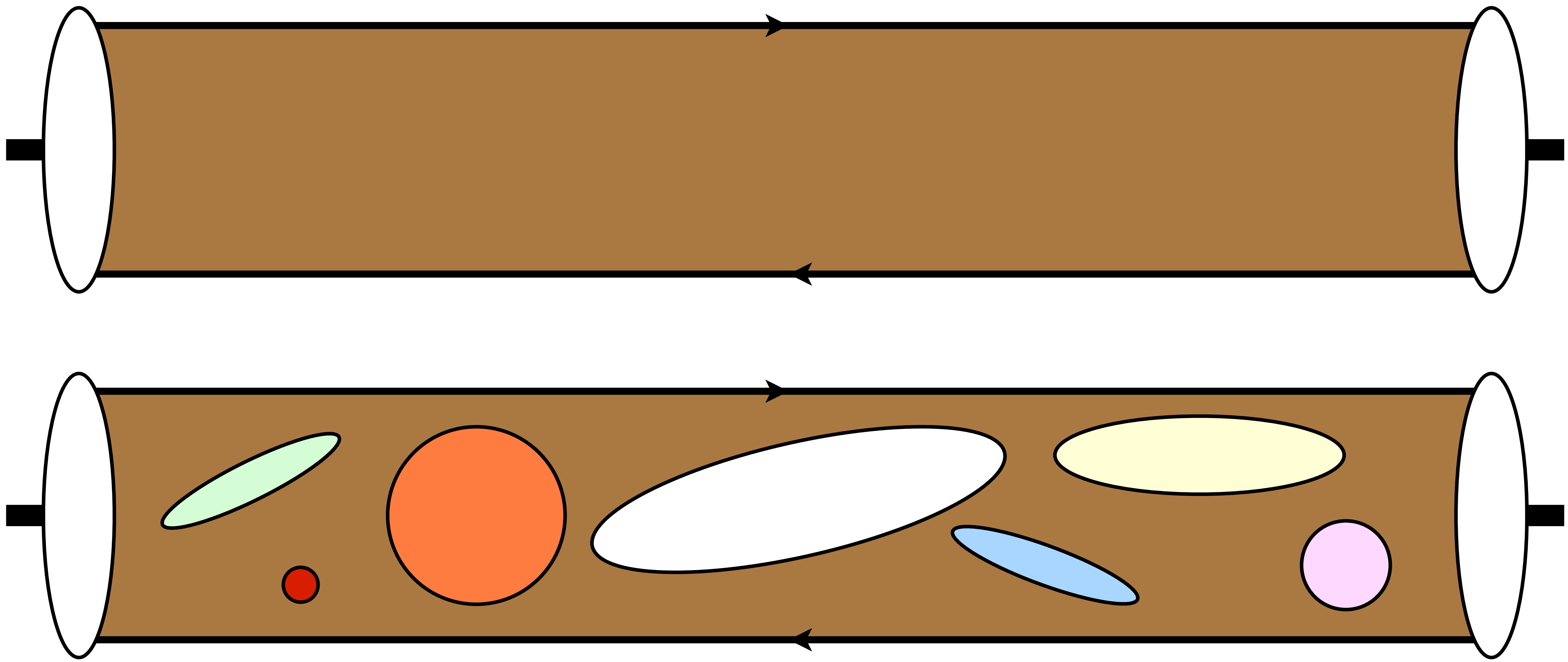
- The contribution of sea quarks is represented mathematically by the determinant of a huge matrix:

  - computationally most demanding step in lattice QCD;

  - quenching: set $\det = 1$ (in early days also called *valence* approximation); notation: $n_f = N$ means N sea quarks with $\det \neq 1$.

  - a dielectric idea: the brown muck is a frequency-dependent medium, approximated by a constant (absorbed into bare g_0^2).

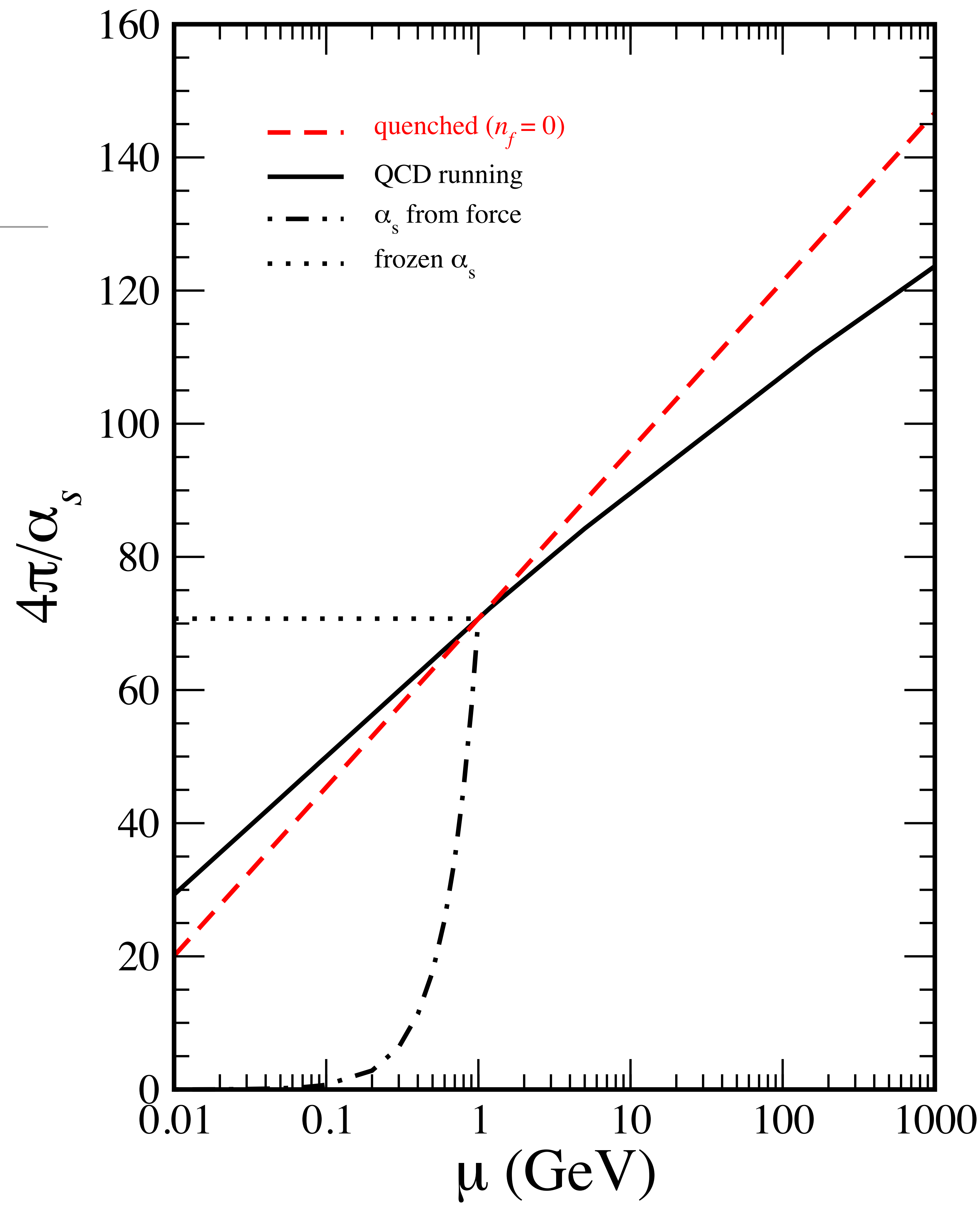
Valence quarks, sea quarks, & gluons



Quenched approximation appears in other contexts, *e.g.*, Schwinger-Dyson equations in ladder approximation.

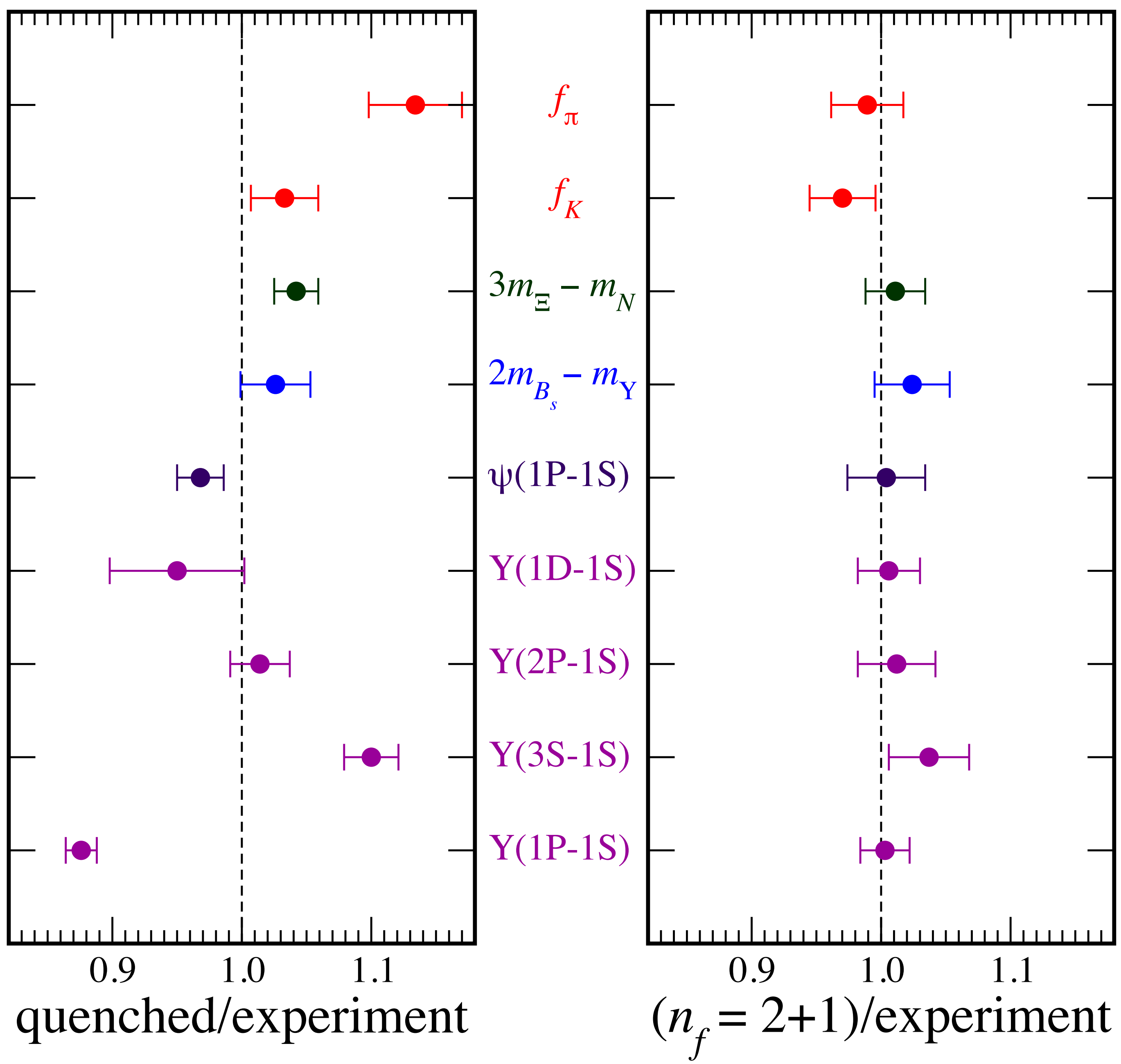
Quenching

- Short distances (large μ):
  - universally incorrect running;
  - arguably unimportant or correctable.
- Long distances (small μ):
  - non-universal IR effects, *e.g.*, $\alpha_s(1/r) = -3r^2F(r)/4$ or “frozen” coupling.



Quenched vs. 2+1 Sea Quarks

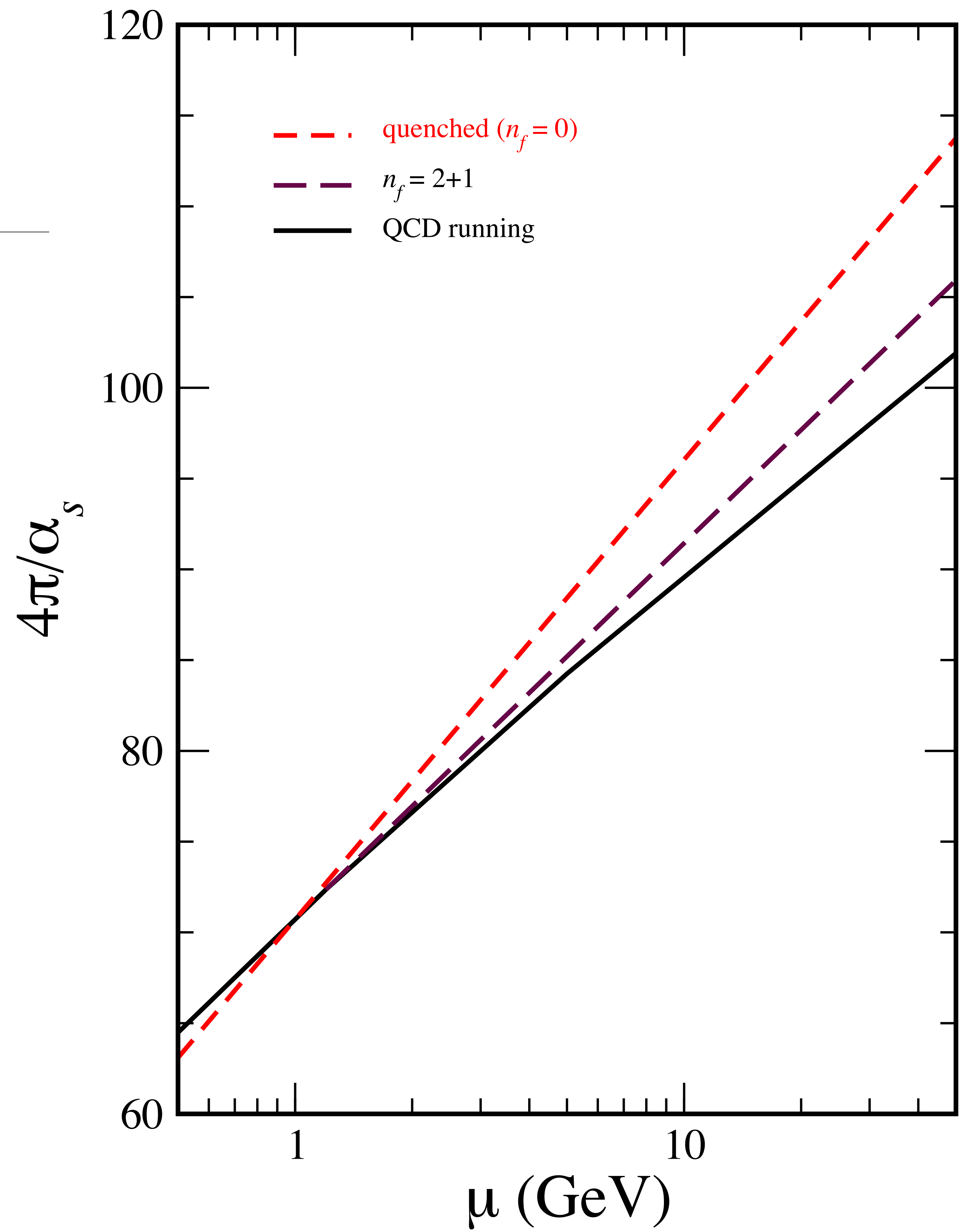
HPQCD, MILC, Fermilab Lattice, hep-lat/0304004



- a = 0.12 & 0.09 fm
- O(a^2) improved
- FAT7 smearing
- $2m_l < m_q < m_s$
- π, K, Υ(2S) input

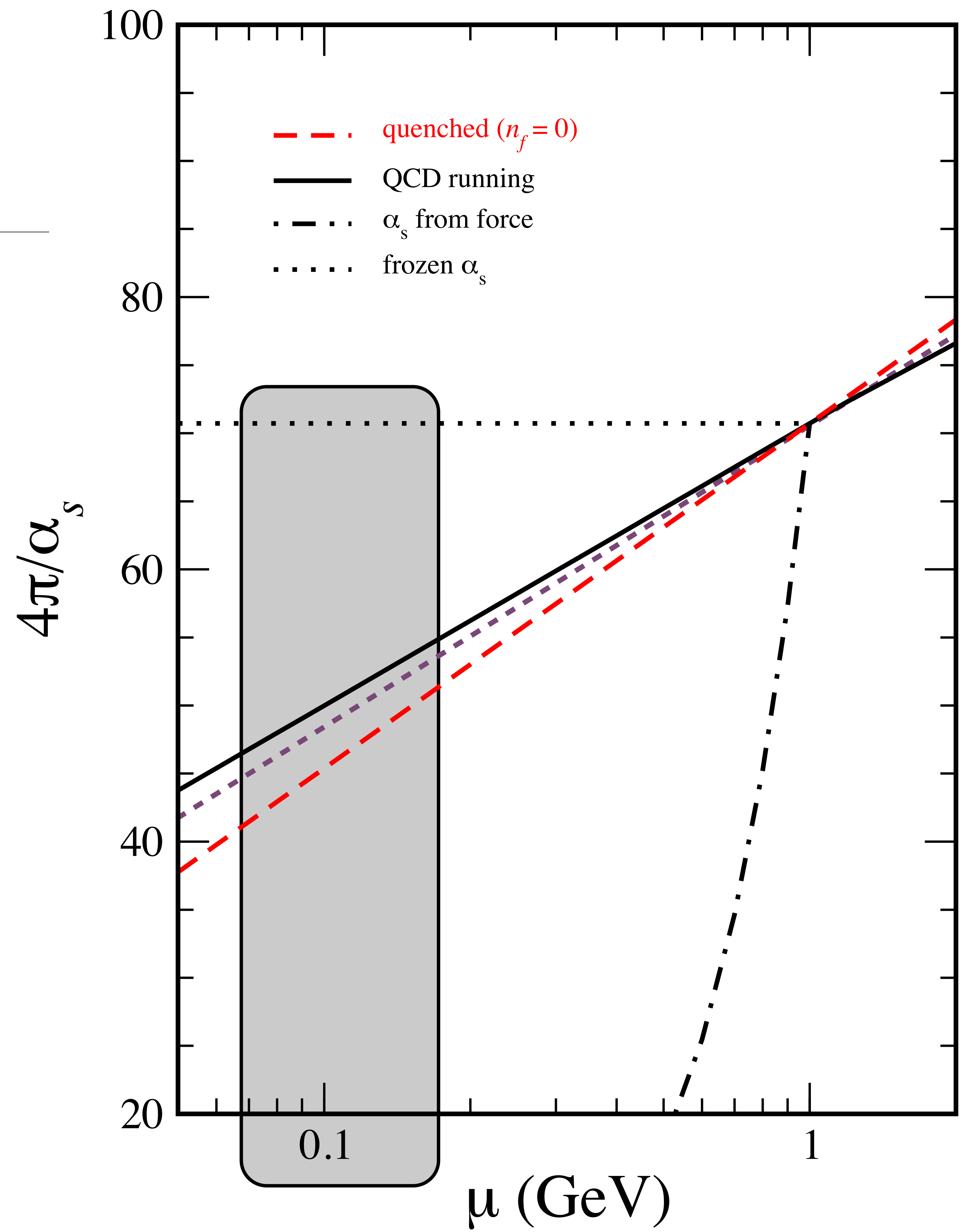
Quenching charm

- Charm threshold lies above nonperturbative regime:
  - expand $\det(\not{D} + m_c)$ in $\not{D}/m_c$;
  - leads to $F_{\mu\nu}F^{\mu\nu}$ action;
  - so shifts α_s (as is customary for b, t);
  - real error $\propto \alpha_s \times (\Lambda/m_c)^2$.



Quenching strange

- Strange threshold lies in nonperturbative regime:
  - $n_f = 2$ better than $n_f = 0$;
  - still hard to estimate;
  - sometimes ~5%;
  - sometimes no change, *e.g.*, Ω mass.



- Caution: many, if not most, quenched calculations contain no estimates of the associated error.

- Caution: many, if not most, $n_f = 2$ calculations contain no estimates of the error associated with quenching the strange sea.
  - Statement of philosophy: “I see no sensible and reliable way to estimate the effect of the strange sea. Many examples show practically no influence from it. This is a puzzle .”
  - “Differences [in f_{Ds} with $n_f = 2$ and $n_f = 2{+}1$] could be due to other effects.”
  - We report; you decide.

- Caution: no $n_f = 2{+}1$ calculations contain hard estimates of the error associated with omitting the charmed sea: 0.1% or 0.5% or 1% or 5%?

Rooted Staggered Fermions

- Many 2+1 calculations use staggered fermions [Susskind, 1977] for quarks.

- Computationally swiftest way to incorporate determinant, but extra four-fold replication of species "tastes". *Ansatz* [Hamber *et al.*, 1983]:

$$\left[\underset{4}{\det}(\not{D}_{\text{stag}}+m)\right]^{1/4} \stackrel{?}{\doteq} \underset{1}{\det}(\not{D}+m)$$

- Extra tastes lead at $a \neq 0$ to violations of unitarity, reducing to physical system as $a \to 0$, handled with a version of chiral perturbation theory:

  - if correct, error incorporated into "chiral extrapolation error";

  - if incorrect, the error is, like quenching, non-quantitative (*caveat emptor*: there are several incorrect arguments about incorrectness).

Semi-quantitative Errors

Errors Estimated Semi-quantitatively

- Sometimes the (numerical) data are insufficient to estimate robustly an uncertainty:
    - the statistical quality is not good enough;
    - the range of parameters is not wide enough;
    - try this, that, and the other fit; cogitate; repeat.
- These cases are a limiting case of errors estimated *quantitatively*, so are discussed later in the talk.

Errors Estimated Semi-quantitatively 2

- Perturbative matching (a class of discretization effect):
  - estimate error from truncating PT with the same "reliability" as in continuum pQCD;
  - multi-loop perturbative lattice gauge theory is daunting.
  - nonperturbative matching, where feasible, fixes this.
- Heavy-quark discretization effects:
  - theory says $\alpha_s^{l+1} b_i^{[l+1]}(am_q) a^n \langle O_i \rangle \sim \alpha_s^{l+1} b_i^{[l+1]}(am_q)(a\Lambda)^n$;
  - for each LHQ action, know asymptotics of b_i, but not $b_i^{[l+1]}(am_q)$.

Quantitative Errors: Statistics

Lattice Gauge Theory

$$\langle \bullet \rangle = \frac{1}{Z}\int \mathcal{D}U \; \mathcal{D}\psi \, \mathcal{D}\bar{\psi} \; \exp(-S)\,[\bullet]$$

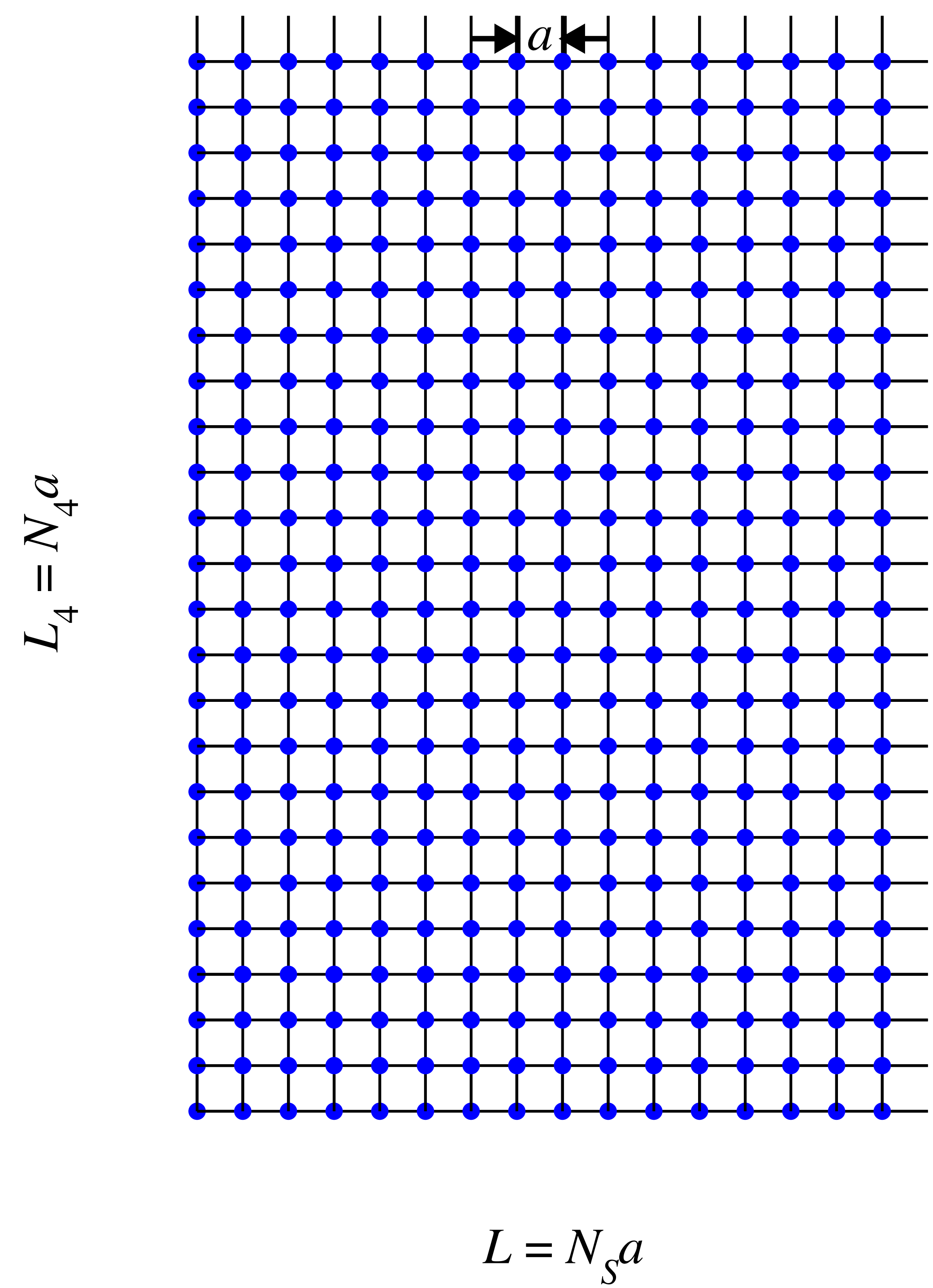
MC   hand

$$= \frac{1}{Z}\int \mathcal{D}U \; \det(\not{D} + m) \exp(-S)\,[\bullet']$$

- Infinite continuum: uncountably many d.o.f.

- Infinite lattice: countably many; used to define QCD

- Finite lattice: can evaluate integrals on a computer; dimension ~ 10^8



Monte Carlo Integration with Importance Sampling

- Estimate integral as a sum over randomly chosen configurations of U:

$$\langle \bullet \rangle = \frac{1}{Z} \int \mathcal{D}U \det(\not{D} + m) \exp(-S) [\bullet'] \approx \frac{1}{C} \sum_{c=0}^{C-1} \bullet' [U^{(c)}]$$

where $\{U^{(c)}\}$ is distributed with probability density $\det(\not{D} + m) \exp(-S)$; often called "simulation," although this may be an abuse of language.

- Sum converges to desired result as ensemble size $C \to \infty$.

- With $C < \infty$, statistical errors and correlations between, say, $G(t)$ and $G(t+a)$.

n-Point Functions

~~Correlators~~ Yield Masses & Matrix Elements

- Two-point functions for masses $\pi(t) = \bar{\psi}_u \gamma_5 S \psi_d$:

$$G(t) = \langle \pi(t) \pi^\dagger(0) \rangle = \sum_n |\langle 0|\hat{\pi}|\pi_n\rangle|^2 \exp(-m_{\pi_n} t)$$

- Two-point functions for decay constants:

$$\langle J(t) \pi^\dagger(0) \rangle = \sum_n \langle 0|\hat{J}|\pi_n\rangle \langle \pi_n|\hat{\pi}^\dagger|0\rangle \exp(-m_{\pi_n} t)$$

- Three-point functions for form factors, mixing:

$$\langle \pi(t) J(u) B^\dagger(0) \rangle = \sum_{mn} \langle 0|\hat{\pi}|\pi_m\rangle \langle \pi_n|\hat{J}|B_m\rangle \langle B_m|\hat{B}^\dagger|0\rangle \times \exp[-m_{\pi_n}(t-u) - m_{B_m} u]$$

Central Limit Theorem

- Thought simulation: generate many ensembles of size C. Observables $\langle \bullet \rangle$ are Gaussian-distributed around true value, with $\langle \sigma^2 \rangle \sim C^{-1}$.
- Inefficient use of computer to generate many ensembles (make ensemble bigger; run at smaller lattice spacing; different sea quark masses; …).
- Generate pseudo-ensembles from original ensemble:
  - jackknife: omit each individual configuration in turn (or adjacent pairs, trios, etc.) and repeat averaging and fitting; estimate error from spread;
  - bootstrap: draw individual configurations at random, allowing repeats, to make as many pseudo-ensembles of size C as you want.

- A further advantage of Jackknife and Bootstrap is that they can be wrapped around an arbitrarily complicated analysis.

- In this way, correlations in the statistical error can be propagated to ensemble properties with a non-linear relation to the *n*-point functions.

    - masses are an example: $m \approx \ln(G_{t+a}/G_t)$;

    - as a consequence, everything else, from amputating legs with Ze^{-mt}.

- Thus, each mass or matrix element is an ordered pair—(central value, bootstrap distribution); understand all following arithmetic this way.

Error Bars and Covariance Matrix

- Errors on the *n*-point functions are determined from the ensemble:

$$\sigma^2(t) = \frac{1}{C-1}\left[\langle G(t)G(t)\rangle - \langle G(t)\rangle^2\right]$$

- Similarly for the covariance matrix:

$$\sigma^2(t_1,t_2) = \frac{1}{C-1}\left[\langle G(t_1)G(t_2)\rangle - \langle G(t_1)\rangle\langle G(t_2)\rangle\right]$$

- Minimize

$$\chi^2(\boldsymbol{m},\boldsymbol{Z}) = \sum_{t_1,t_2}\left[G(t_1) - \sum_n Z_n e^{-m_n t_1}\right]\sigma^{-2}(t_1,t_2)\left[G(t_2) - \sum_n Z_n e^{-m_n t_2}\right]$$

to obtain masses, m_n, and matrix elements, Z_n, for few lowest-lying states.

Data Reduction

- Computing a hadron n-point function from a lattice gauge field represents a huge data reduction.
- We consider an ensemble pretty big if it has 500 (independent) configurations.
- Reduce to a function with 20 discrete values: $20 \ll 500 \times 20/4$.
- But now fit, using the statistical correlation among the function values: alas, $20 \times 20 \not\ll 500 \times 20/4$.
- Now correlate this function with others (*e.g.*, one for mass, one for matrix element; several final-state momenta for a form factor).

Constrained Curve-Fitting

- The fits to towers of states are the first of many fits, in which a series is a "theorem" (here a genuine theorem).

- Figuring out fit ranges and where to truncate is a bit of a dark art.

- More recently, some groups have been assigning Bayesian priors to higher terms in the series, fitting

$$\chi^2_{\text{aug}} = \chi^2(\boldsymbol{G}|\{\boldsymbol{Z},\boldsymbol{m}\}) + \chi^2(\{\boldsymbol{Z},\boldsymbol{m}\})$$

- Anything with "Bayesian" in it can lead to long discussions, often fruitless.

- Key observation is that *decisions where to truncate* are priors: indeed extreme ones, $\delta(Z_n = 0)$ or $\delta(m_n = \infty)$, $n > s$. *Choosing fit range* is prior on data.

Quantitative Errors: Tuning

The Lagrangian

- 1 + n_f + 1 parameters:

fiducial observable

$$\mathcal{L}_{\text{QCD}} = \frac{1}{g_0^2}\,\text{tr}[F_{\mu\nu}F^{\mu\nu}]$$
r_1 or m_Ω or $\Upsilon(2S\text{-}1S)$...

$$- \sum_f \bar{\psi}_f(\not{D} + m_f)\psi_f$$
$m_\pi, m_K, m_{J/\psi}, m_\Upsilon, \ldots.$

$$+ \frac{i\theta}{32\pi^2}\varepsilon^{\mu\nu\rho\sigma}\,\text{tr}[F_{\mu\nu}F_{\rho\sigma}]$$
$\theta = 0.$

  - Fixing the parameters is essential step, *not* a loss of predictivity.
  - Length scale r_1: $r_1^2 F(r_1) = 1$ (from static potential): need other inputs too.
  - Statistical and systematic uncertainties propagate from fiducials to others.

Quantitative Errors: Effective Field Theories

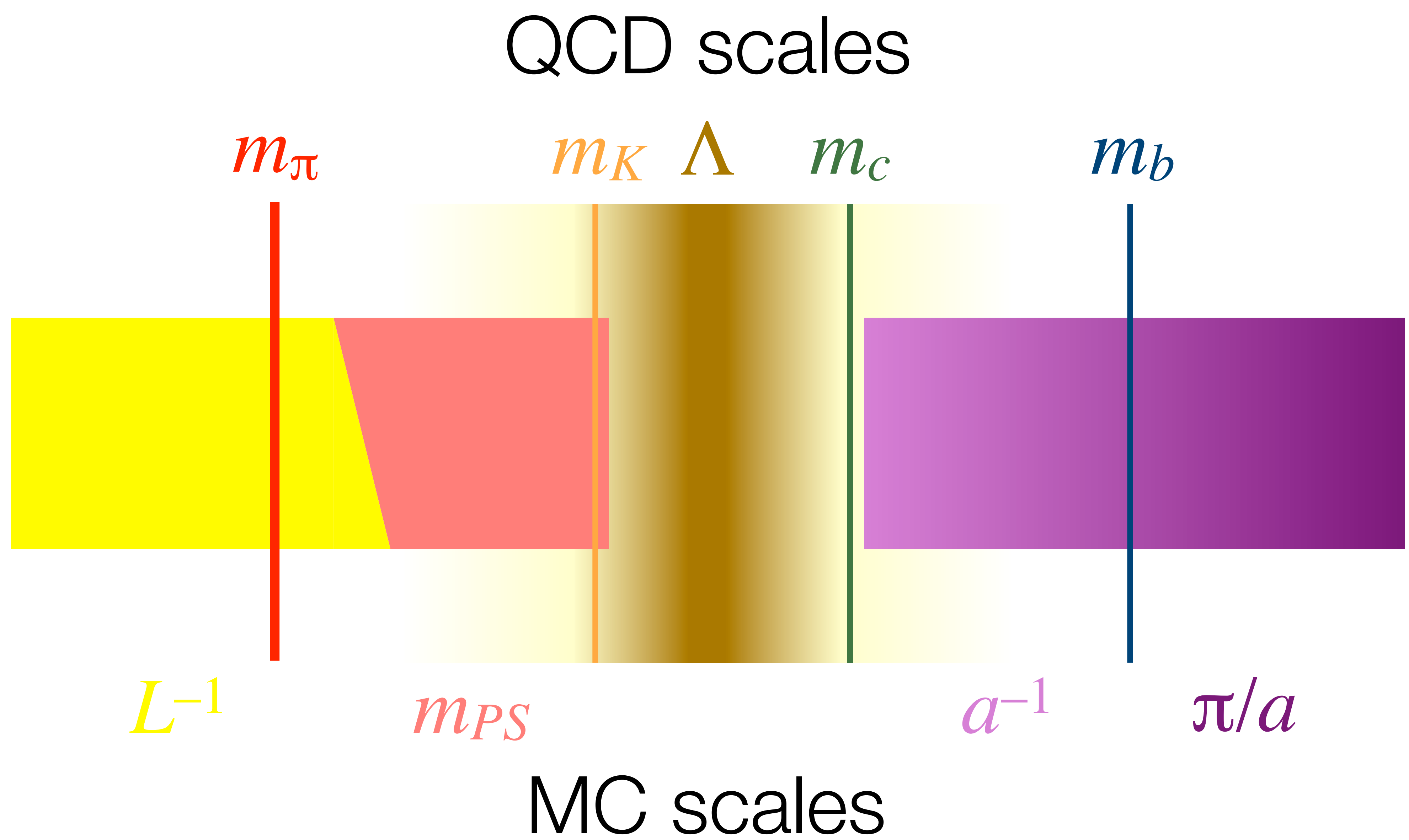
review: hep-lat/0205021

Yesterday's Output is Today's Input

- After running the Monte Carlo a few years, accumulating zillions of files with *n*-point functions, and spending a couple months fitting them into zillions more files with masses and matrix element, the real work can begin.

- The (numerical) data are generated for a sequence of
  - lattice spacing;
  - spatial volume;
  - light quark masses;
  - heavy quark masses.

Many Scales in Lattice QCD



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- The (numerical) data are generated for a sequence of

  - lattice spacing;
  - light quark masses;
  - spatial volume;
  - heavy quark masses;

  - $a \to 0$ with Symanzik EFT;
  - $m_\pi^2 \to (140\ \mathrm{MeV})^2$ with chiral PT;
  - massive hadrons $\oplus$ χPT;
  - HQET and NRQCD.

Symanzik Effective Field Theory

- An outgrowth of the "Callan-Symanzik equation"

$$\frac{d\alpha_s(\mu^2)}{d\mu^2} = -\beta_0\alpha_s^2(\mu^2) - \beta_1\alpha_s^3(\mu^2) - \cdots$$

  is Symanzik's theory of cutoff effects.

- Applied to lattice gauge theory (*e.g.*, QCD)

$$\mathcal{L}_{\text{LGT}} \doteq \mathcal{L}_{\text{Sym}} = \mathcal{L}_{\text{QCD}} + \sum_i a^{\dim \mathcal{L}_i - 4} \mathcal{K}_i(g^2, ma; \mu)\mathcal{L}_i$$

  where RHS is a *continuum* field theory with extra operators to describe the cutoff effects. Pronounce $\doteq$ as "has the same physics as".

- Data in computer: $\mathcal{L}_{\text{LGT}}$. Analysis tool: $\mathcal{L}_{\text{Sym}}$.

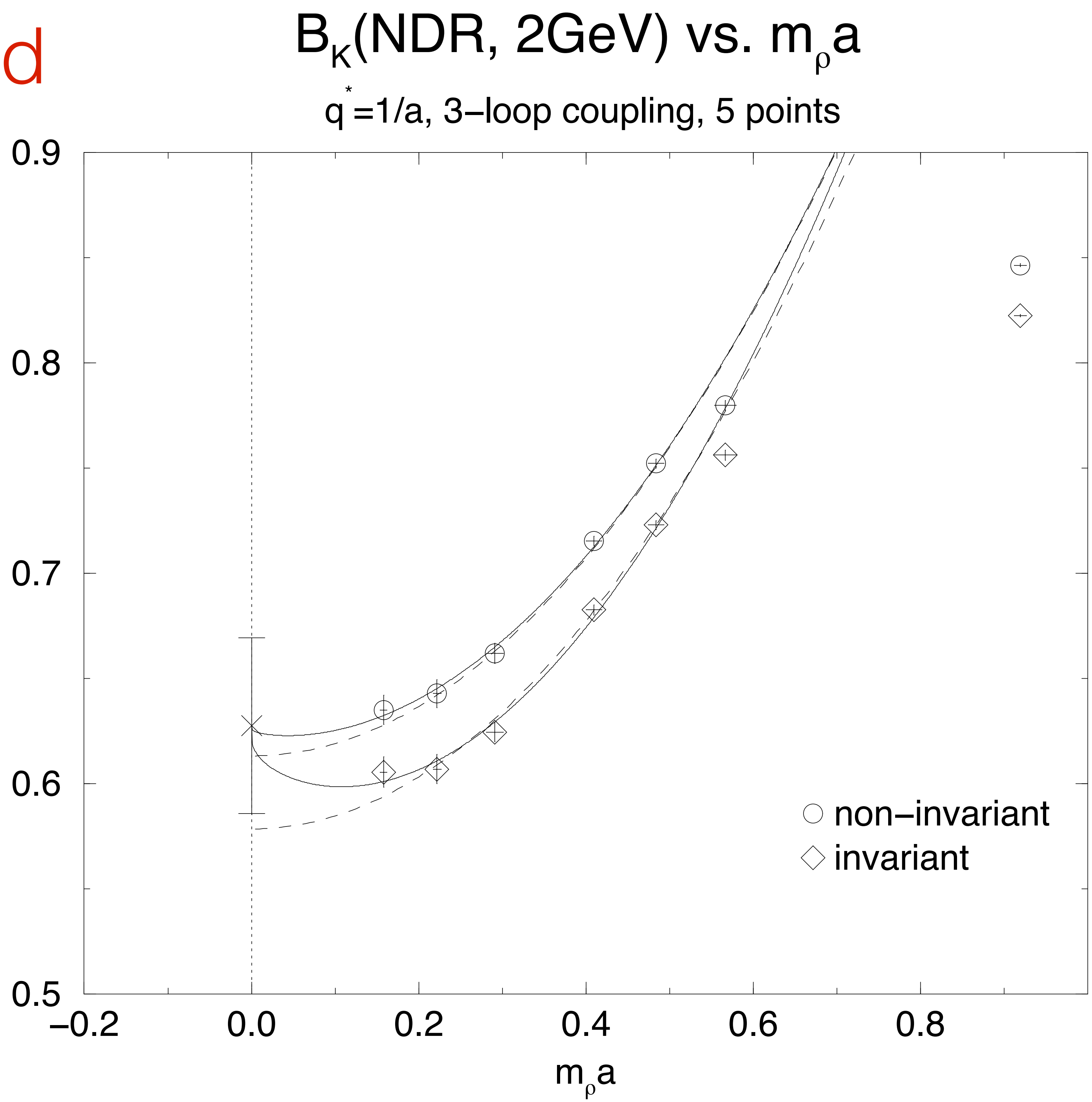
Symanzik Effective Field Theory 2

- The Symanzik LE$\mathcal{L}$ helps in (at least) three ways:
  - a semi-quantitative estimate of discretization effects—$a^n\langle\mathcal{L}_i\rangle \sim (a\Lambda)^n$;
  - a theorem-based strategy for continuum extrapolation: a^n (beware the anomalous dimension in $\mathcal{K}_i$!);
  - a program (the "Symanzik improvement program") for reducing lattice-spacing dependence: if you can reduce the leading $\mathcal{K}_i$ in one observable, it is reduced for all observables:
    - perturbative—$\mathcal{K}_i \sim \alpha_s^{l+1}$; nonperturbative—$\mathcal{K}_i \sim a$.

Exceptional Continuum Extrapolation: B_K

JLQCD, hep-lat/9710073

quenched



Chiral Perturbation Theory

- Chiral perturbation theory [Weinberg, Gasser & Leutwyler] is a Lagrangian formulation of current algebra.

- A nice physical picture is to think of this as a description of the pion cloud surrounding every hadron:

$$\mathcal{L}_{\text{QCD or Sym}} \doteq \mathcal{L}_{\chi\text{PT}}$$

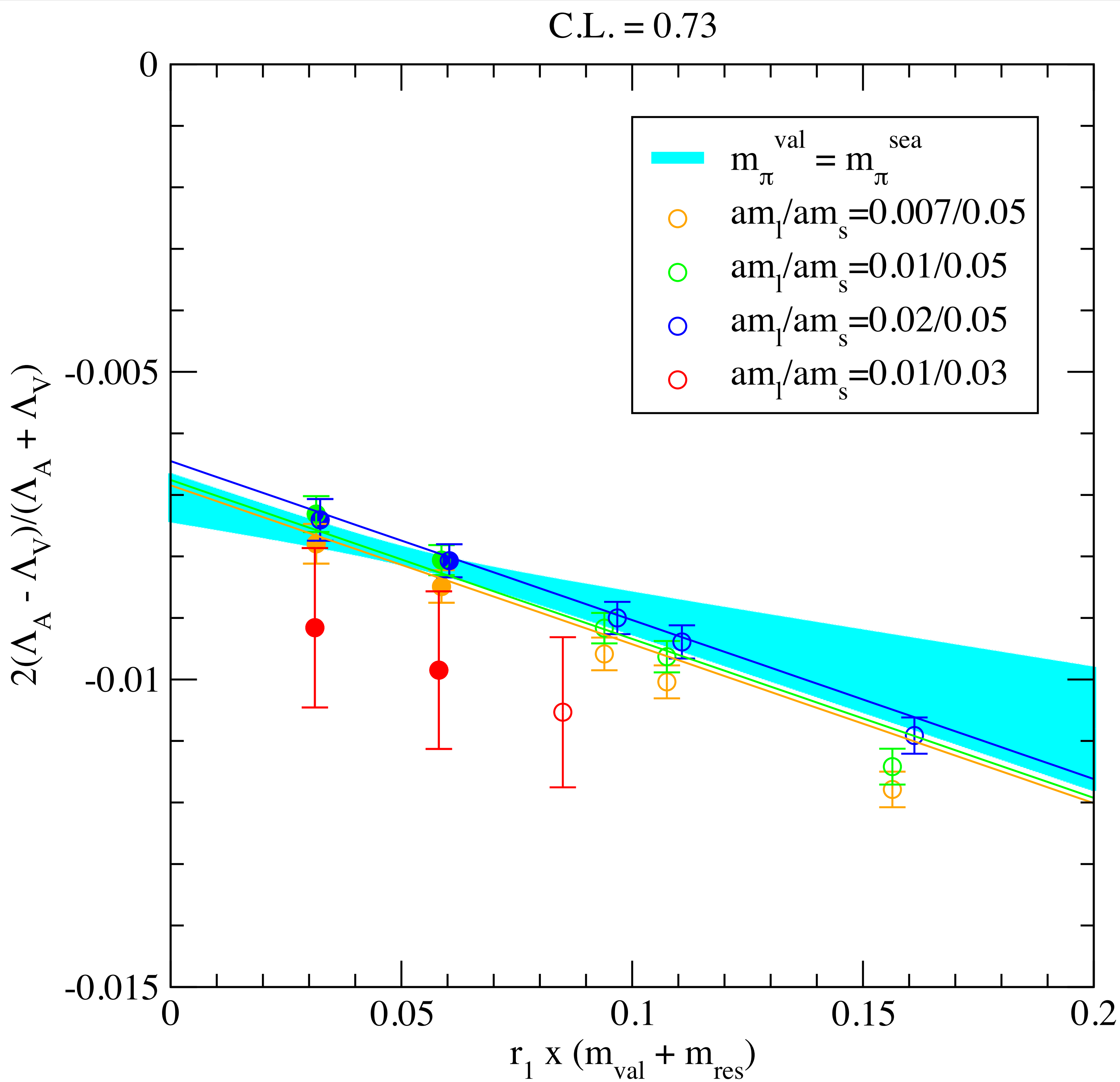
  where the LHS is a QFT of quarks and gluons, and the RHS is a QFT of pions (and, possibly, other hadrons).

- Theoretically efficient: QCD's approximate chiral symmetries constrain the interactions on the RHS. Unconstrained: the couplings on the RHS.

- RHS can include (symmetry-breaking) terms to describe cutoff effects.

Typical Chiral Extrapolation: B_K

Aubin, Laiho, Van de Water, arXiv:0905.3947



Finite-Volume Effects as Error

- All indications (*i.e.*, experiment, LGT) are that QCD is a massive field theory.

- A general result for static quantities in massive field theories trapped in a finite box with $e^{i\theta}$-periodic boundary conditions [Lüscher, 1985]:

$$M_n(\infty) - M_n(L) \sim g_{n\pi} \exp\left(-\mathrm{const}\, m_\pi L\right)$$

  so once $m_\pi L \gtrsim 4$ or so, these effects are negligible.

- For two-body states, the situation is more complicated, and more interesting.

- Volume-dependent energy shift encode information about resonance widths and final-state phase shifts (*cf.* Norman Christ's talk, tomorrow).

Finite-Volume Effects as Technique

- When finite-volume effects are well-described by χPT, the finite-volume, even small-volume, data can be used to determine the couplings of the Gasser-Leutwyler Lagrangian.

- Several regimes:

  - *p*-regime: $1 \sim Lm_\pi \ll L\Lambda$ (usual pion cloud, squeezed a bit);

  - ε-regime: $Lm_\pi \ll 1 \ll L\Lambda$ (pion zero-mode nonperturbative).

- Review: S. Necco, arXiv:0901.4257.

Heavy Quarks

- For heavy quarks on current lattices, $m_Q a \not\ll 1$, worry about errors ~$(m_Q a)^n$.

- Heavy-quark symmetry to the rescue:

$$\begin{aligned}\mathcal{L}_{\text{QCD}} \doteq \mathcal{L}_{\text{HQ}} &= \sum_s m_Q^{-s} \sum_i \mathcal{C}_i^{(s)}(\mu)\mathcal{O}_i^{(s)}(\mu) \\ &= \bar{h}_v \left[v \cdot D + mZ_m(\mu)\right] h_v + \frac{\bar{h}_v D_\perp^2 h}{2mZ_m(\mu)} + \cdots\end{aligned}$$

$$\begin{aligned}\mathcal{L}_{\text{LGT}} \doteq \mathcal{L}_{\text{HQ}(a)} &= \sum_s m_Q^{-s} \sum_i \mathcal{C}_i^{(s)}(m_Q a, c_i; \mu)\mathcal{O}_i^{(s)}(\mu) \\ &= \bar{h}_v \left[v \cdot D + m_1(\mu)\right] h_v + \frac{\bar{h}_v D_\perp^2 h_v}{2m_2(\mu)} + \cdots \\ &= \sum_s a^s \sum_i \bar{\mathcal{C}}_i^{(s)}(m_Q a, c_i; \mu)\mathcal{O}_i^{(s)}(\mu)\end{aligned}$$

Heavy-quark Effective Field Theory

- Using HQET as a theory of cutoff effects helps in (at least) three ways:
  - a semi-quantitative estimate of discretization effects—$b_i a^n \langle O_i \rangle \sim (a\Lambda)^n$;
  - a theorem-based strategy for continuum extrapolation, although the $m_Q a$ dependence of the b_i makes this less easy than in Symanzik; *cf*. Claude Bernard's talk for an example with priors.
  - a program for reducing lattice-spacing dependence: if you can reduce the leading b_i in one observable, it is reduced for all observables:
    - perturbative— $b_i \sim \alpha_s^{l+1}$; nonperturbative— $b_i \sim a$ or $1/m_Q$.

Summary

A Very Good Error Budget

(one omission)

stats

tuning

chiral

continuum

$$\Delta_q = 2m_{Dq} - m_{\eta c}$$

	f_K/f_π	f_K	f_π	f_{D_s}/f_D	f_{D_s}	f_D	Δ_s/Δ_d
r_1 uncerty.	0.3	1.1	1.4	0.4	1.0	1.4	0.7
a^2 extrap.	0.2	0.2	0.2	0.4	0.5	0.6	0.5
Finite vol.	0.4	0.4	0.8	0.3	0.1	0.3	0.1
$m_{u/d}$ extrap.	0.2	0.3	0.4	0.2	0.3	0.4	0.2
Stat. errors	0.2	0.4	0.5	0.5	0.6	0.7	0.6
m_s evoln.	0.1	0.1	0.1	0.3	0.3	0.3	0.5
m_d, QED, etc.	0.0	0.0	0.0	0.1	0.0	0.1	0.5
Total %	0.6	1.3	1.7	0.9	1.3	1.8	1.2

charmed sea $\ll 0.5\%$?

Questions?