Introduction to Lattice QCD

Understanding Uncertainty Budgets

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Lattice Meets Experiment
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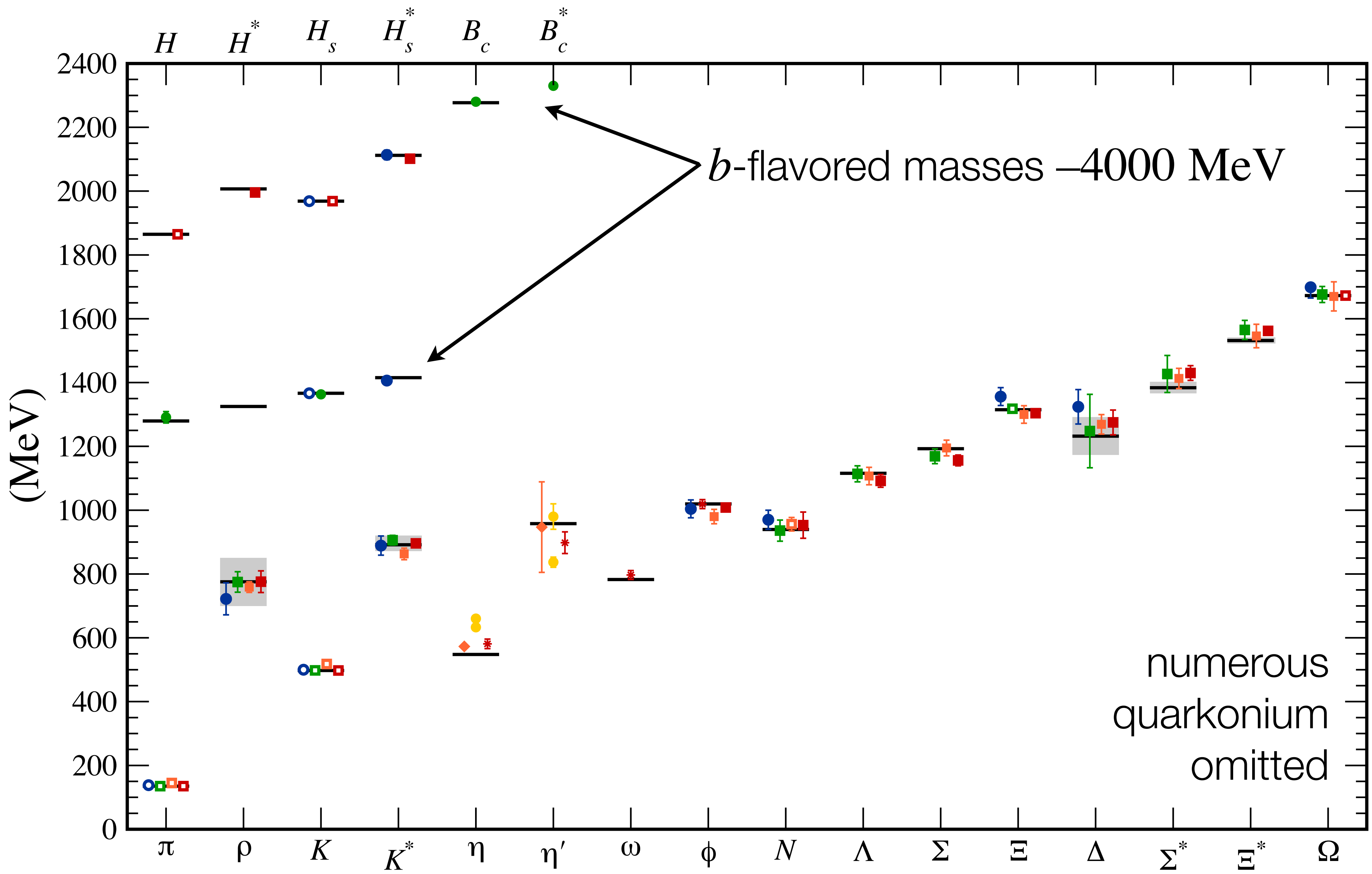
QCD Hadron Spectrum

$\pi \ldots \Omega$: BMW, MILC, PACS-CS, QCDSF;
η-η': RBC, UKQCD, Hadron Spectrum (ω);
D, B: Fermilab, HPQCD, Mohler&Woloshyn



Quark Flavor Physics: Then and Now

Quantity	CKM element	Present expt. error	2007 forecast lattice error	Present lattice error	2018 lattice error
f_K/f_π	$\|V_{us}\|$	0.2%	0.5%	0.5%	0.15%
$f_+^{K\pi}(0)$	$\|V_{us}\|$	0.2%	–	0.5%	0.2%
f_D	$\|V_{cd}\|$	4.3%	5%	2%	$< 1\%$
f_{D_s}	$\|V_{cs}\|$	2.1%	5%	2%	$< 1\%$
$D \to \pi\ell\nu$	$\|V_{cd}\|$	2.6%	–	4.4%	2%
$D \to K\ell\nu$	$\|V_{cs}\|$	1.1%	–	2.5%	1%
$B \to D^*\ell\nu$	$\|V_{cb}\|$	1.3%	–	1.8%	$< 1\%$
$B \to \pi\ell\nu$	$\|V_{ub}\|$	4.1%	–	8.7%	2%
f_B	$\|V_{ub}\|$	9%	–	2.5%	$< 1\%$
ξ	$\|V_{ts}/V_{td}\|$	0.4%	2–4%	4%	$< 1\%$
ΔM_s	$\|V_{ts}V_{tb}\|^2$	0.24%	7–12%	11%	5%
B_K	$\mathrm{Im}(V_{td}^2)$	0.5%	3.5–6%	1.3%	$< 1\%$

Quantum Mechanics with Path Integrals

- Heisenberg & Pauli [Z. Phys. 56, 1 (1929)] used a spatial lattice and took a limit to set up canonical commutation relations for QED:

$$[p_i, q_j] = i\hbar\delta_{ij} \to [p_x, q_y] = i\hbar\delta(x-y)$$

- Feynman showed that QM amplitudes can be expressed as “path” integrals [RMP 20, 367 (1948)]:

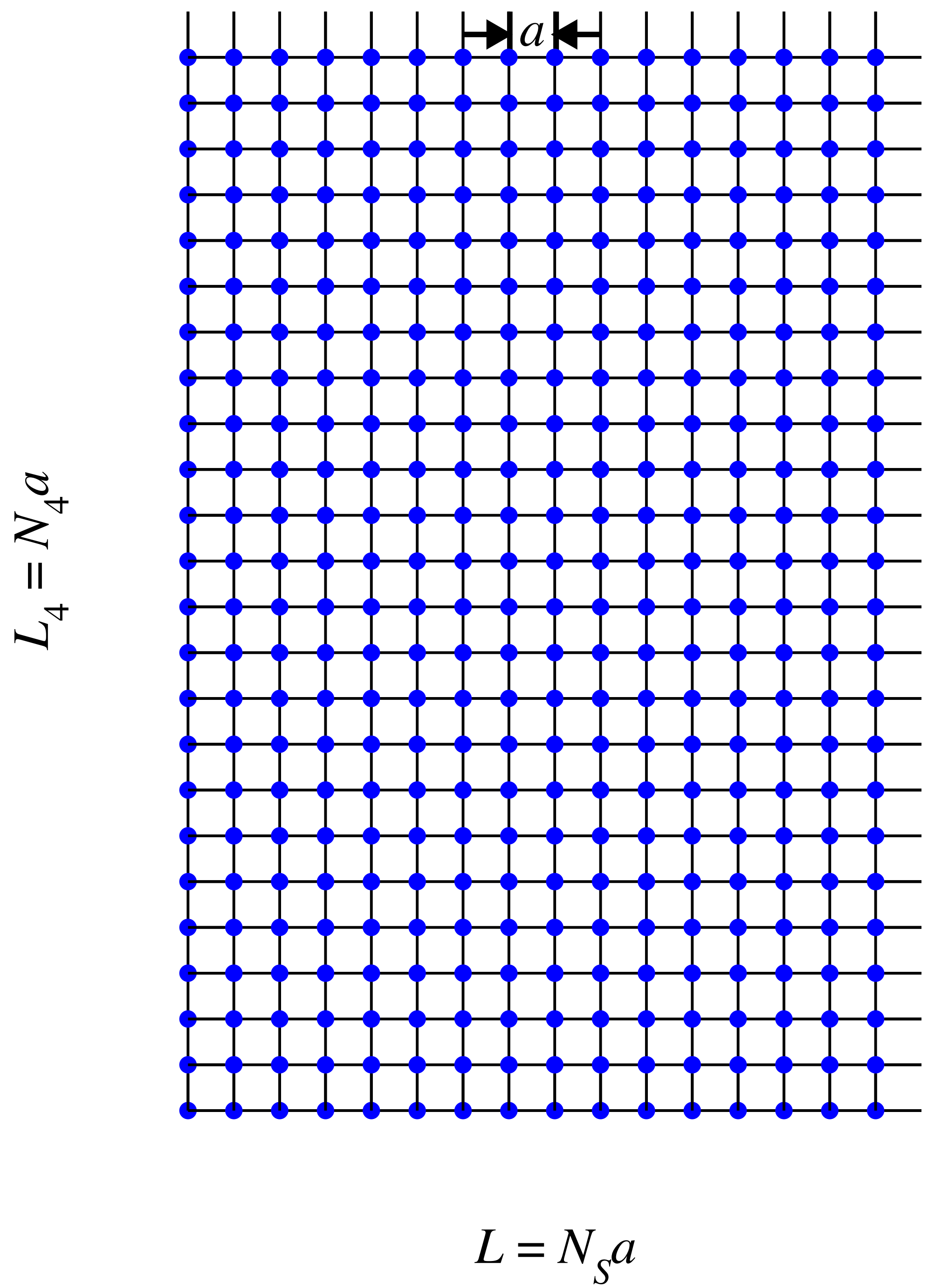
$$\langle x(t)|x(0)\rangle = \lim_{N\to\infty} \int \prod_{i=1}^{N-1} dx_i e^{iSt/N}$$

- Kenneth Wilson combined the two technical steps with (his) renormalization theory to define gauge theories, such as QCD, on a space-time lattice [PRD 10, 2445 (1974)]. This is lattice gauge theory.

Lattice Field Theory =: Quantum Field Theory

- Infinite continuum: uncountably many d.o.f.
- Infinite lattice: countably many; used to define quantum field theory.
- Finite lattice: can evaluate integrals on a computer; dimension ~ 10^8.
- Monte Carlo with importance sampling:

$$\begin{aligned}\langle \bullet \rangle &= \frac{1}{Z}\int \mathcal{D}U \;\; \mathcal{D}\psi\, \mathcal{D}\bar{\psi} \;\; \exp(-S)\,[\bullet] \\ &= \frac{1}{Z}\int \mathcal{D}U \det(\not{D}+m)\exp(-S)\,[\bullet']\end{aligned}$$



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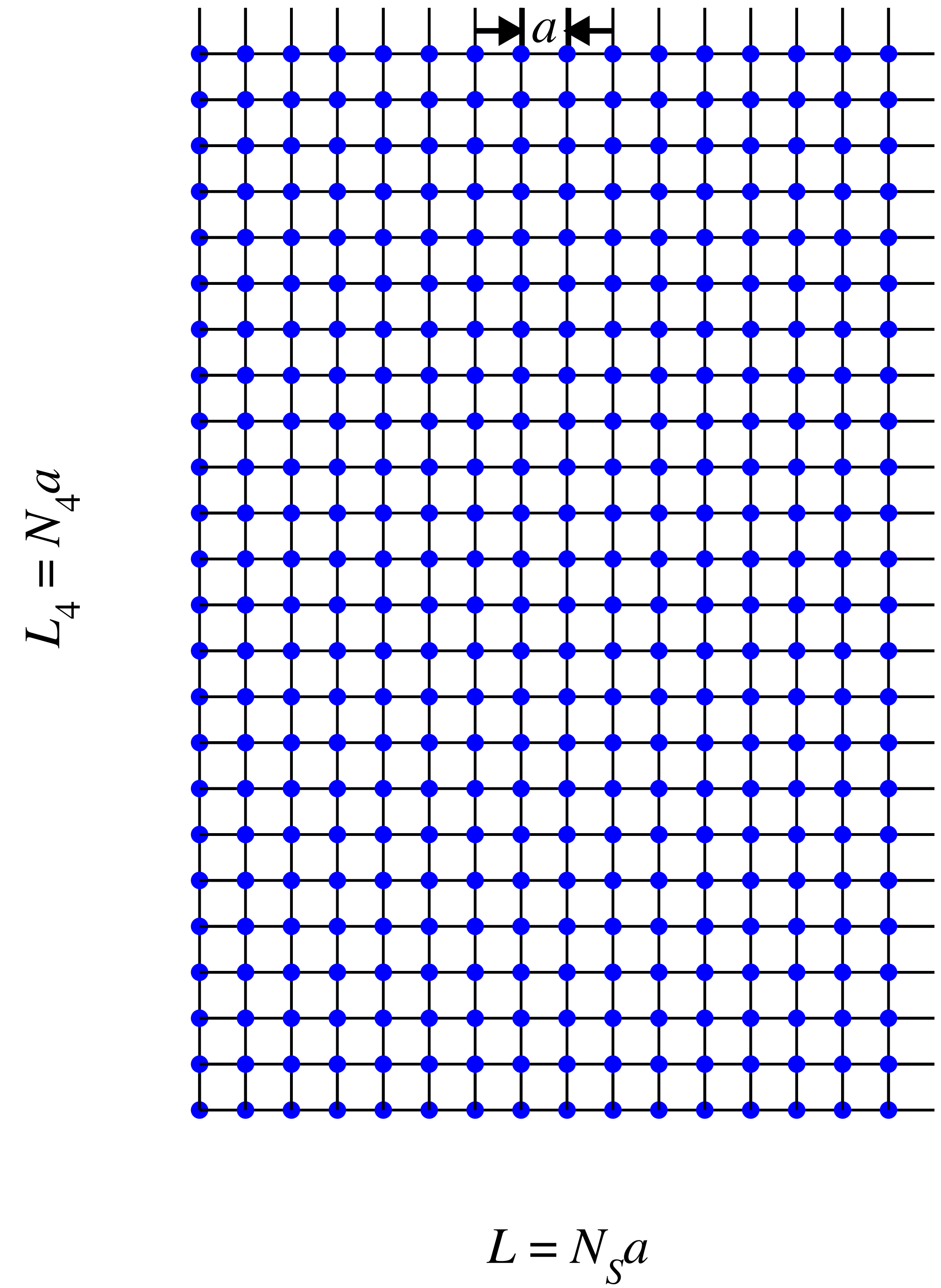

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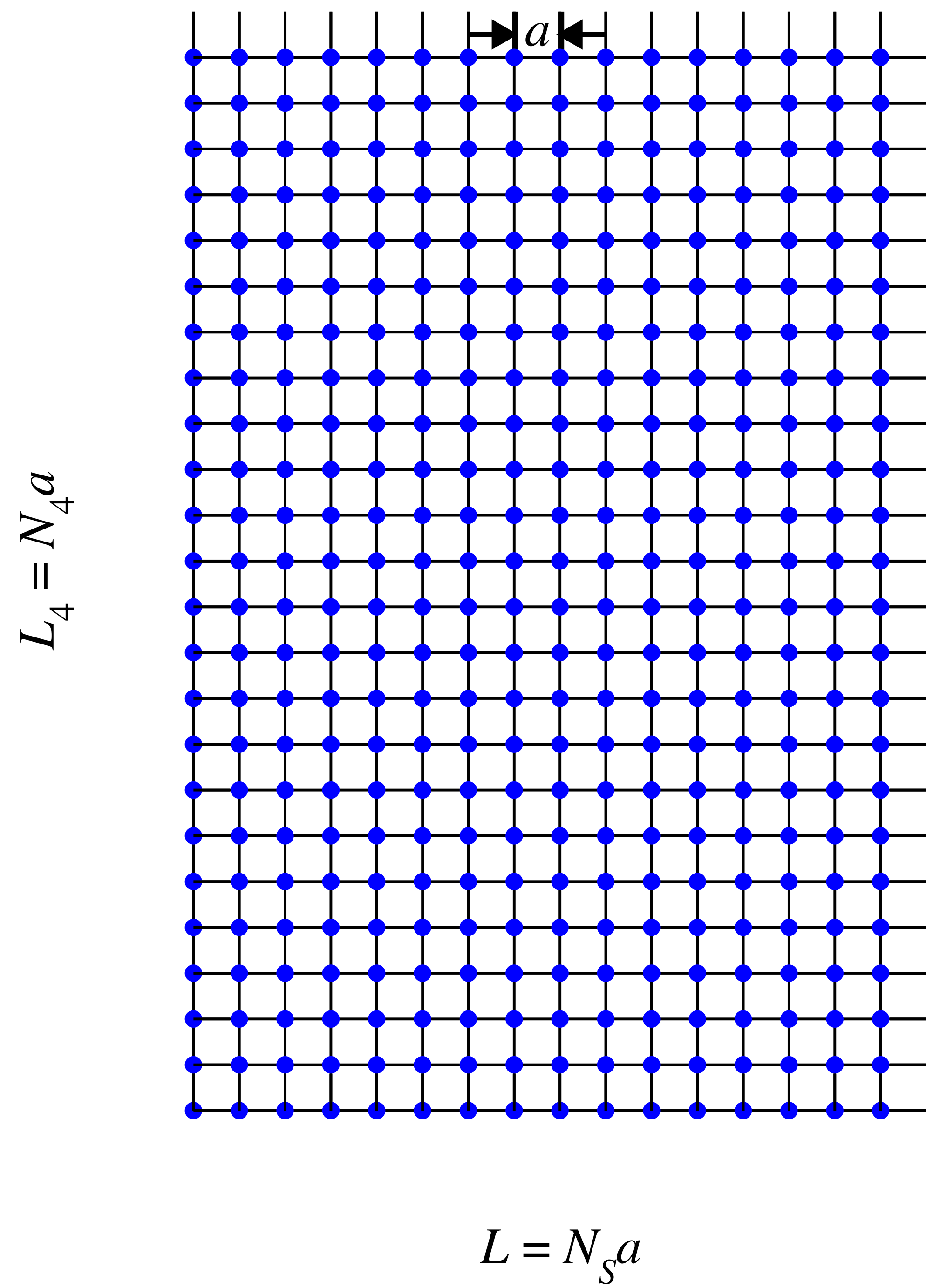

n-Point Functions Yield Masses & Matrix Elements

- Two-point functions for masses $\pi(t) = \bar{\psi}_u \gamma^5 \psi_d$:

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

- Two-point functions for decay constants:

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

- Three-point functions for form factors, mixing:

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

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.

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 $\alpha_s^{l+1} b_i^{[l+1]}(am_q)\, a^n\langle O_i\rangle$, with $a^n\langle O_i\rangle \sim (a\Lambda)^n$;
  - for each LHQ action, know asymptotics of $b_i(am_q)$, but that's it.

Quantitative Errors: Statistics

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 $G(t+a)$.

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: $G(t) \approx Z\mathrm{e}^{-mt}Z \Rightarrow m \approx \ln[G(t)/G(t+a)]$;

  - as a consequence, everything else, from amputating legs with $Z\mathrm{e}^{-mt}$.

- 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 estimated 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.

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.

- Some groups assign 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 a fit range* is prior on data.

Quantitative Errors: Tuning

The Lagrangian

- 1 + n_f + 1 parameters:

$$\begin{aligned}\mathcal{L}_{\mathrm{QCD}} &= \frac{1}{g_0^2}\,\mathrm{tr}[F_{\mu\nu}F^{\mu\nu}] \\ &- \sum_f \bar{\psi}_f(\not{D}+m_f)\psi_f \\ &+ \frac{i\theta}{32\pi^2}\,\varepsilon^{\mu\nu\rho\sigma}\,\mathrm{tr}[F_{\mu\nu}F_{\rho\sigma}]\end{aligned}$$

- Fixing the parameters is essential step, *not* a loss of predictivity.
- Length scale w_0 is defined via a diffusion equation; r_1 via QQ potential.
- Statistical and systematic uncertainties propagate from fiducials to others.

The Lagrangian

- 1 + n_f + 1 parameters:

<u>fiducial observable</u>

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w_0, r_1, m_Ω, or Υ(2S-1S)...

m_π, m_K, $m_{J/\psi}$, m_Υ, ...

$\theta = 0$.

- Fixing the parameters is essential step, *not* a loss of predictivity.

- Length scale w_0 is defined via a diffusion equation; r_1 via QQ potential.

- 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.

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  - lattice spacing;

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  - heavy quark masses—more recently, $m_c a \ll 1$, and even $m_b a \ll 1$.

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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"

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

- is an effective field theory to study cutoff effects of lattice field theories:

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

  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: $\mathscr{L}_{\mathsf{LGT}}$. Analysis tool: $\mathscr{L}_{\mathsf{Sym}}$.

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—$\mathcal{K}_i \sim a$.

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:

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

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

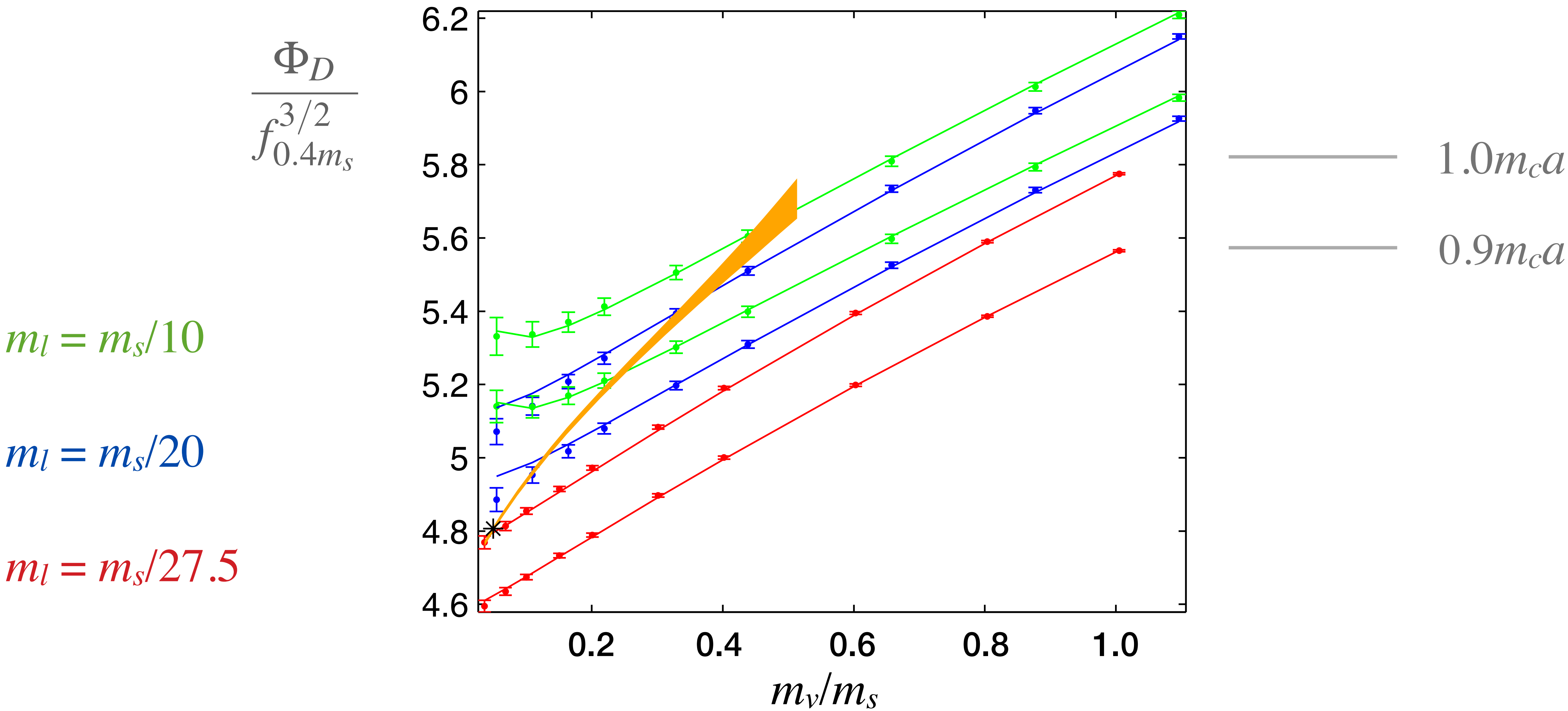
- Theoretically efficient: QCD's approximate chiral symmetries constrain the interactions on the RHS, and fits to LHS data yield the couplings on the RHS.

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

Recent Chiral Extrapolation: f_D

Bazavov *et al.*, arXiv:1312.0149

$$\Phi_D = f_D\sqrt{M_D}$$



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]:

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

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.

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: $1 \sim L m_\pi \ll L\Lambda$ (usual pion cloud, squeezed a bit);

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

- Review: K. Splittorff, arXiv:1211.1803.

Heavy Quarks

- For heavy quarks on current lattices, $m_Q a \not\ll 1$, worry about errors ~$(m_Q a)^n$.
- Heavy-quark physics to the rescue:

$$\mathscr{L}_{\mathrm{QCD}} \doteq \mathscr{L}_{\mathrm{HQ}} = \sum_s m_Q^{-s} \sum_i \mathscr{C}_i^{(s)}(\mu)\mathscr{O}_i^{(s)}(\mu)$$

same

$$= \bar{h}[v \cdot D + mZ_m(\mu)]h + \frac{\bar{h}D_\perp^2 h}{2mZ_m(\mu)} + \cdots$$

$$\mathscr{L}_{\mathrm{LGT}} \doteq \mathscr{L}_{\mathrm{HQ}(a)} = \sum_s m_Q^{-s} \sum_i \mathscr{C}_i^{(s)}(m_Q a, c_i; \mu)\mathscr{O}_i^{(s)}(\mu)$$

$$= \bar{h}[v \cdot D + m_1(\mu)]h + \frac{\bar{h}D_\perp^2 h}{2m_2(\mu)} + \cdots$$

$$= \sum_s a^s \sum_i \overline{\mathscr{C}}_i^{(s)}(m_Q a, c_i; \mu)\mathscr{O}_i^{(s)}(\mu)$$

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; in arXiv:1112.3051 these effects are treated 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

Bailey *et al.*, arXiv:1403.0635

stats
tuning
chiral
continuum

any omissions?

Uncertainty	$h_{A_1}(1)$
Statistics	0.4%
Scale (r_1) error	0.1%
χPT fits	0.5%
$g_{D^*D\pi}$	0.3%
Discretization errors	1.0%
Perturbation theory	0.4%
Isospin	0.1%
Total	1.4%

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$|V_{cb}|$

Current Status

⟨Lattice|  |Experiment⟩

- We compute (best) matrix elements with 1 or (harder) 2 particles in the initial state, and 0, 1, or 2 in the final state, mediated by a local operator.
- Meson matrix elements have made huge strides over the past ten years.
- We expect that nucleon matrix elements, as well as quantities such as those needed for muon g–2, to make similar strides in the next ten years.

Questions?