Uncertainty Quantification in Lattice Quantum Chromodynamics

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Uncertainty quantification in lattice gauge theory

- Some of the most important searches for the effects of new physics on known particles are limited by the uncertainty analysis in lattice QCD calculations.
    - Understanding the significance of these searches depends on understanding the solidity of the uncertainty quantification.
    - Most of the human work in good lattice QCD is in the determination of the uncertainties.
- Code and method verification issues are similar in lattice gauge simulations to other large-scale simulations.
- "Validation" is a bit different.
    - The equations of quantum chromodynamics are taken to be established laws of nature.

- There are several classes of lattice gauge calculations with respect to UQ.
  - Uncertainties are in principle under control and small. (Stable hadron masses, leptonic decay constants, semileptonic decays, ...)
  - Uncertainties are in principle under control, but large. (ε'/ε.)
  - Uncertainties are under unknown control and the reliability of a qualitative answer is desired. (Is chiral symmetry broken in a strongly coupled beyond-the-Standard-Model theory.)
  - Methods don't exist. (Finite chemical potential in dense nuclear matter, ...)
- I'll discuss the first class.
  - Dominant errors (finite lattice spacing a, finite volume V, too large quark mass m, ...) governed by calculable physics at large volumes, short distances.
  - Can be estimated with physics calculations.

High Energy Physics

The Standard Model:

- Three forces (strong, weak, and electromagnetic), with coupling strengths:

$$\alpha_{\mathrm{s}},\ \alpha_{\mathrm{w}},\ \alpha_{\mathrm{em}}$$

- Six quark and six lepton masses

$$m_u,\ m_d,\ m_c,\ m_s,\ m_t,\ m_b$$

$$m_e,\ m_\mu,\ m_\tau,\ m_{\nu_1},\ m_{\nu_2},\ m_{\nu_3}$$

- Mixings among the quarks, the Cabibbo-Kobayashi-Maskawa matrix (2008 Nobel Prize), and (as of the last few years) among the leptons:

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \qquad \begin{pmatrix} V_{e\nu_1} & V_{e\nu_2} & V_{e\nu_3} \\ V_{\mu\nu_1} & V_{\mu\nu_2} & V_{\mu\nu_3} \\ V_{\tau\nu_1} & V_{\tau\nu_2} & V_{\tau\nu_3} \end{pmatrix}$$

Where do these parameters come from?
Can we predict them with a more fundamental theory?

High Energy Physics

The Standard Model:

- Three forces (strong, weak, and electromagnetic), with coupling strengths:

$$\boxed{\alpha_\mathrm{s},}\ \alpha_\mathrm{w},\ \alpha_\mathrm{em}$$

Domain of lattice QCD

- Six quark and six lepton masses

$$\boxed{m_u,\ m_d,\ m_c,\ m_s,}\ m_t,\ \boxed{m_b}$$

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The Standard Model accounts for every particle physics experiment performed so far, sometimes to great precision (one part in a billion for the electron anomalous magnetic moment).

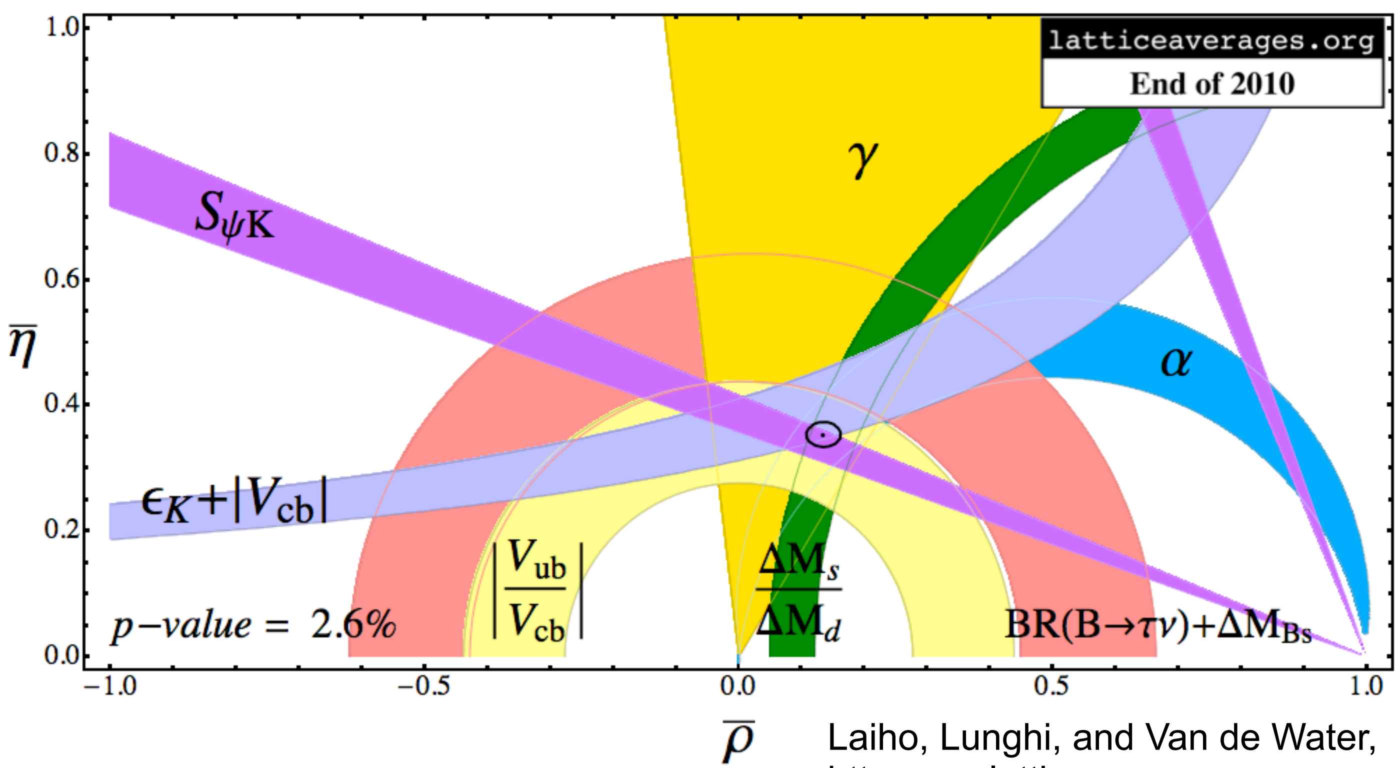
But..
it contains obvious gaps and puzzles

- A mathematically consistent theory cannot be constructed from the currently observed particles.
  - At least one additional, undiscovered particle is required. Is it the ‘’Higgs” boson, or something more complicated?
- Many other puzzles.
- A search for new physics “beyond the Standard Model is the central task of particle physics today.

in SM

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \Rightarrow V = \begin{pmatrix} 1-\lambda^2/2 & \lambda & A\lambda^3(\rho - i\eta) \\ -\lambda & 1-\lambda^2/2 & A\lambda^2 \\ A\lambda^3(1-\rho-i\eta) & -A\lambda^2 & 1 \end{pmatrix} + \mathcal{O}(\lambda^4)$$

In the standard model, the quark mixing matrix is (special) unitary, and determined by four parameters, but
new, beyond-the-standard-model interactions could make them all different.



Laiho, Lunghi, and Van de Water,
http:www.latticeaverages.org.

Determinations of ρ and η are inconsistent at the ~2.5 σ level.
Is it a hint of new physics, or mis-estimated uncertainties from experiment or theory?

Quantum Chromodynamics (QCD)

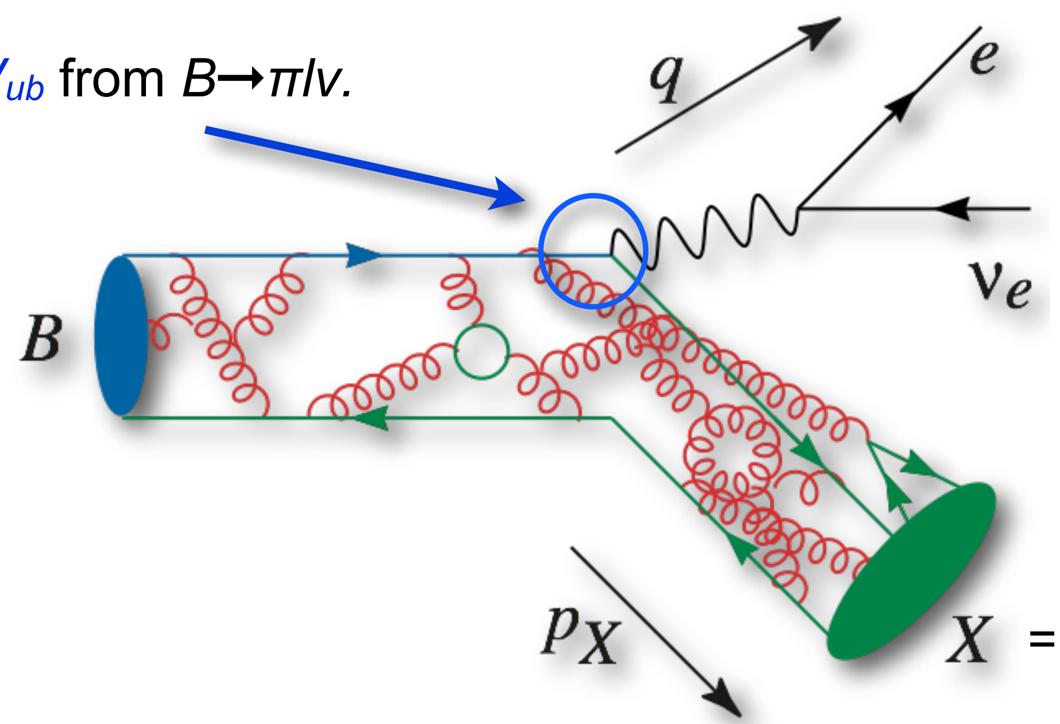
QCD is the theory of quarks and gluons. Quarks and gluons cannot be directly observed because the forces of QCD are strongly interacting.

Quarks are permanently confined inside hadrons, even though they behave as almost free particles at asymptotically high energies.

"Asymptotic freedom", Gross, Politzer, and Wilczek, Nobel Prize, 2004.

Lattice QCD is used to determine the properties of quarks and gluons from the observed properties of hadrons.

Determine V_{ub} from $B \to \pi l \nu$.



= {π, K, ...}

$B \to \pi l \nu$ semileptonic decay

- At short distances and high energies, QCD can be expanded as a series in a small parameter, α_s.
    - “Long distance” = >> size of a proton.
    - “Short distance” = << size of a proton.
    - Analogous to solving the properties of the hydrogen atom in QED as an expansion in α_{em}.
- At the scales of protons and other hadrons (particles containing quarks) this series fails to converge, non-perturbative effects are present, and numerical simulations with lattice QCD are required.

Quantum field theories can be defined by their path integrals.

$$Z = \int d[A_{x\mu}, \psi_x, \overline{\psi}_x] \exp\left(-S(A, \psi, \overline{\psi})\right)$$

gluon gauge fields

fermionic quarks and antiquarks

Independent fields are defined at each point of space-time.

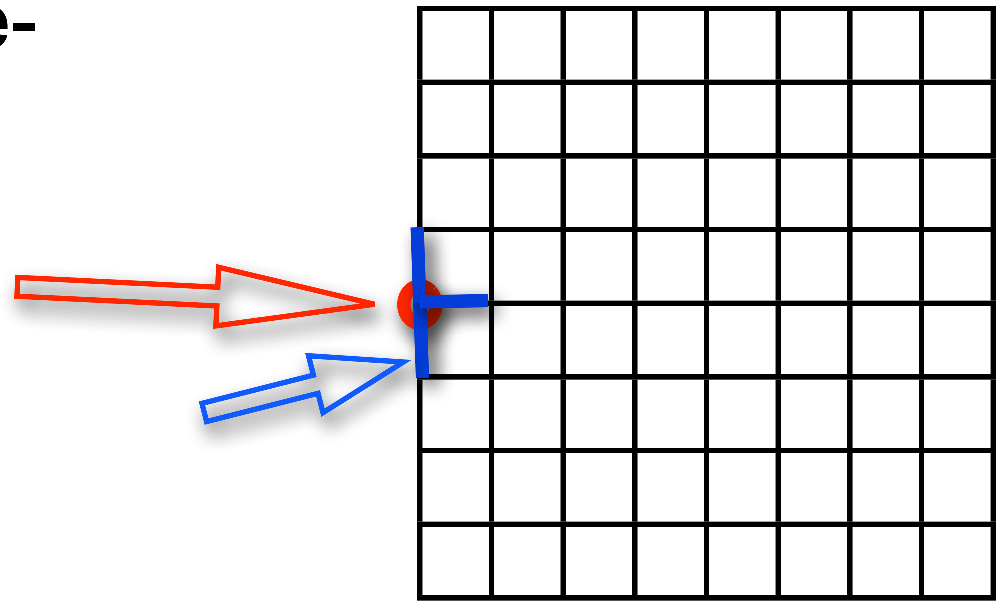
A continuum quantum field theory is in principle defined by an infinite dimensional integral (not a well-defined object).

QFTs must be “regulated”.

Lattice QCD

Approximate the path integral by defining the fields on a four dimensional space-time lattice.

Quarks (ψ) are defined on the sites of the lattice, and gluons (U_μ) on the links.



Monte Carlo methods are used to generate a representative ensemble of gauge fields. Relaxation methods are used to calculate the propagation of quarks through the gauge field.

The discrete Dirac operator

The fundamental operation that consumes the bulk of our cycles is the solution of the Dirac equation on the lattice.

The fundamental component of the Dirac operator is the discrete difference approximation to the first derivative of the quark field on the lattice.

$$\partial_\mu \psi(x) \to \Delta_\mu \psi(x) \approx \frac{1}{2a}(\psi(x+\hat{\mu}a) - \psi(x-\hat{\mu}a)) + \mathcal{O}(a^2)$$

Quarks in QCD come in three colors and four spins.
The color covariant Dirac operator of lattice QCD is

$$D_\mu \gamma_\mu \psi(x) \equiv \frac{1}{2}\left(U_\mu(x)\gamma_\mu \psi(x+\hat{\mu}) - U_\mu^\dagger(x-\hat{\mu})\gamma_\mu \psi(x-\hat{\mu})\right)$$

γ: operates on spin four-vector.

U: SU(3) matrix operates on color three-vector of the quark.

The computational task of lattice QCD

Planned coming generation of gauge ensembles.

Lattice spacing *a (fm)*	Quark mass *ml/ms*	Volume (sites)	Configurations	Ensemble Core-hours (M)
0.12	1/5	24^3*64	1000	3
	1/10	32^3*64	1000	8
	1/27	48^3*64	1000	26
0.09	1/5	32^3*96	1000	10
	1/10	48^3*96	1000	35
	1/27	64^3*96	1000	46
0.06	1/5	48^3*144	1000	38
	1/10	64^3*144	1000	128
	1/27	96^3*144	1000	218
0.045	1/5	64^3*192	1000	135
	1/10	88^3*192	1000	352
	1/27	128^3*192	1000	1083
0.03	1/5	96^3*288	1000	685
				2,770

The largest of these ensembles will require the sustained-petaflop resources which are expected in 2012 at Argonne and Oak Ridge.

Operationally, lattice QCD computations consist of

1) Sampling a representative set of gauge configurations with Monte Carlo methods,

   E.g., the Metropolis method, the hybrid Monte Carlo algorithm, ...
   Consists of one long Markov chain.

2) Calculating the propagation of quarks through the gauge configurations,

   Solve the Dirac equation on each configuration with relaxation methods, e.g., biconjugate gradient algorithm, etc.

3) Constructing hadron correlation functions from the quark propagators.

Verification and validation

Physics may be used to verify methods and codes at several levels.

- Presence of proper symmetries is required.
  - Rotation invariance.
  - Lorentz invariance. ($E^2=m^2+p^2+0\times a^2p^4$.)
  - Gauge invariance.
- Numerical codes may be applied to the short-distance regime, where answers may also be obtained with perturbation theory.
- Comparison of physics results with experiment.

Verification

Gauge invariance.

The physics of lattice gauge theories is invariant under local gauge transformations, configuration by configuration.

Multiplication of fields by arbitrary SU (3) matrix on each site of the lattice.

$$\begin{aligned}\psi(x) &\rightarrow V(x)\psi(x)\\ \overline{\psi}(x) &\rightarrow \overline{\psi}(x)V^\dagger(x)\\ U_\mu(x) &\rightarrow V(x)U_\mu(x)V^\dagger(x+\hat{\mu})\end{aligned}$$

Free quark propagator may be calculated with pencil and paper in momentum space.

Correctness of the sparse matrix inverter aside from gluons (U matrices) may be checked by direct comparison with this result.

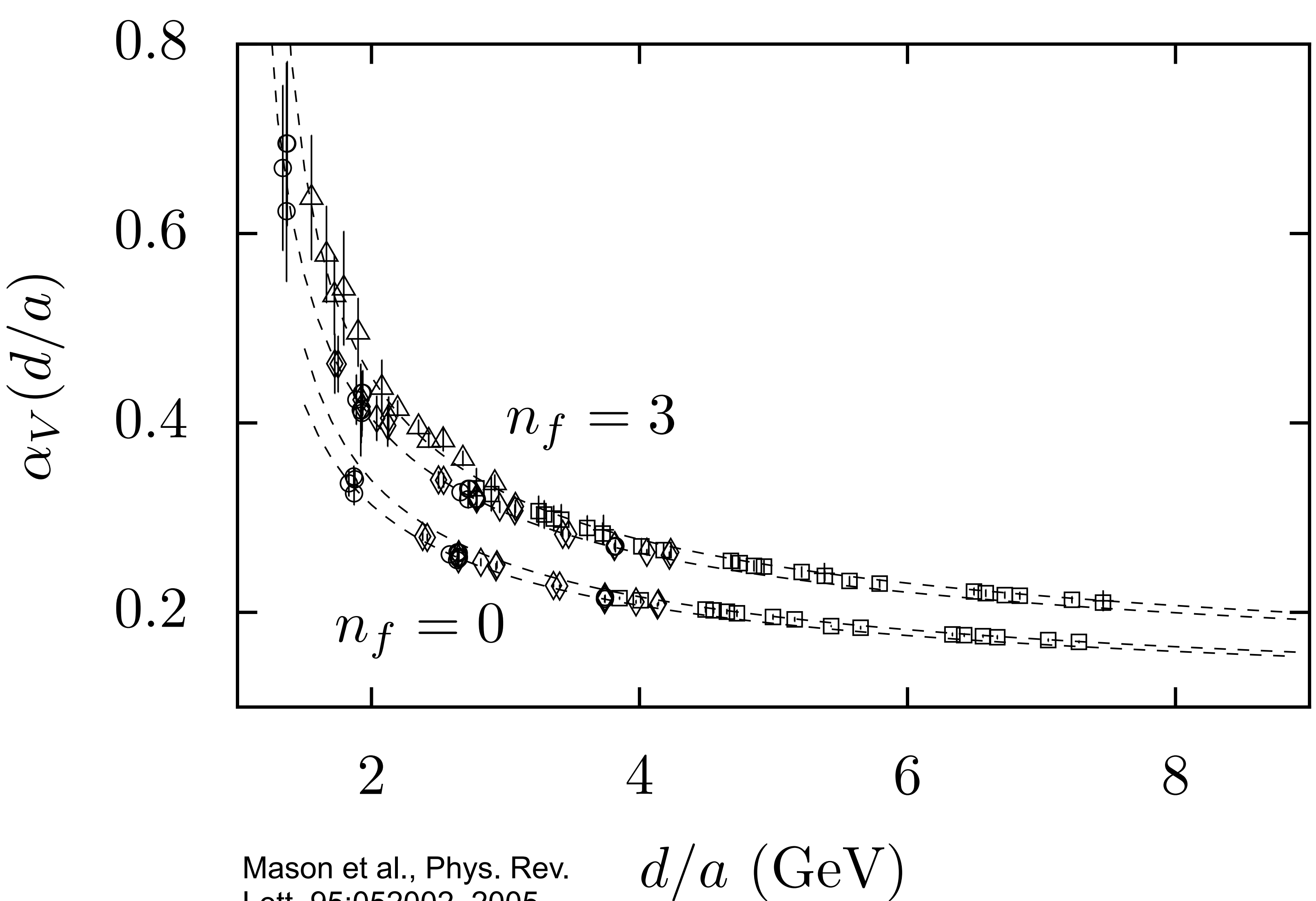
Correctness of the sparse matrix inverter including gluons may be checked by numerically recalculating the free quark propagator after making a random local gauge transformation to a trivial gauge field (U=1).

Free quark propagator should transform: $G(x,y)\rightarrow V(x)G(x,y)V^\dagger(y)$,

Hadron two-point functions, $G_\pi(x,y)=\mathrm{Tr}\ G(x,y)G(y,x)$ are gauge invariant.

Verification

Comparison of Monte Carlo code with perturbation theory at short distances.



Mason et al., Phys. Rev. Lett. 95:052002, 2005.

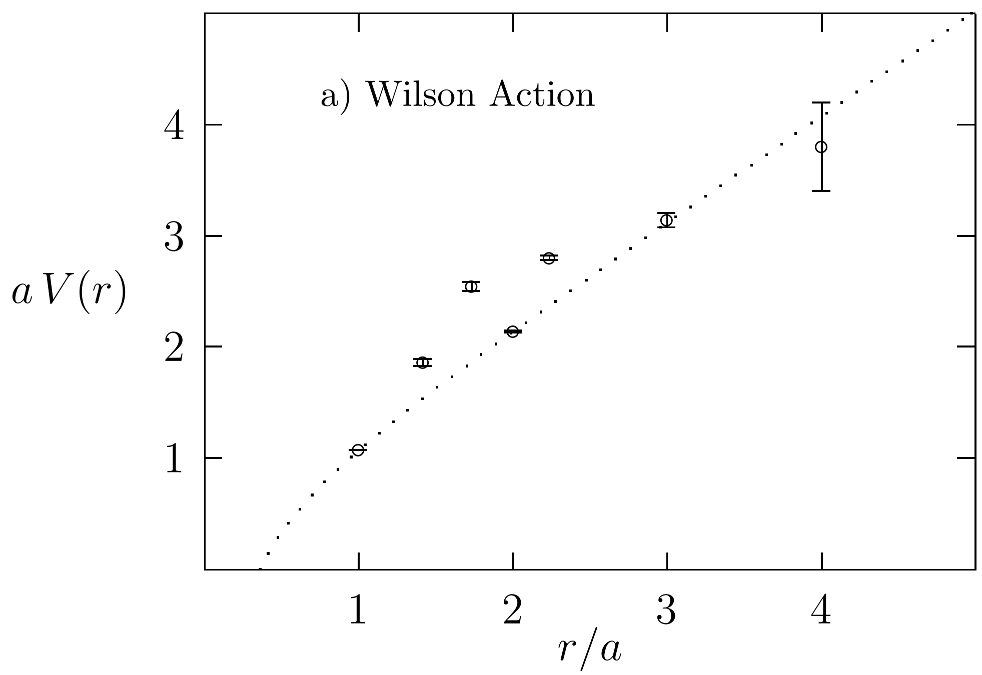
Short distance, high energy ⟶

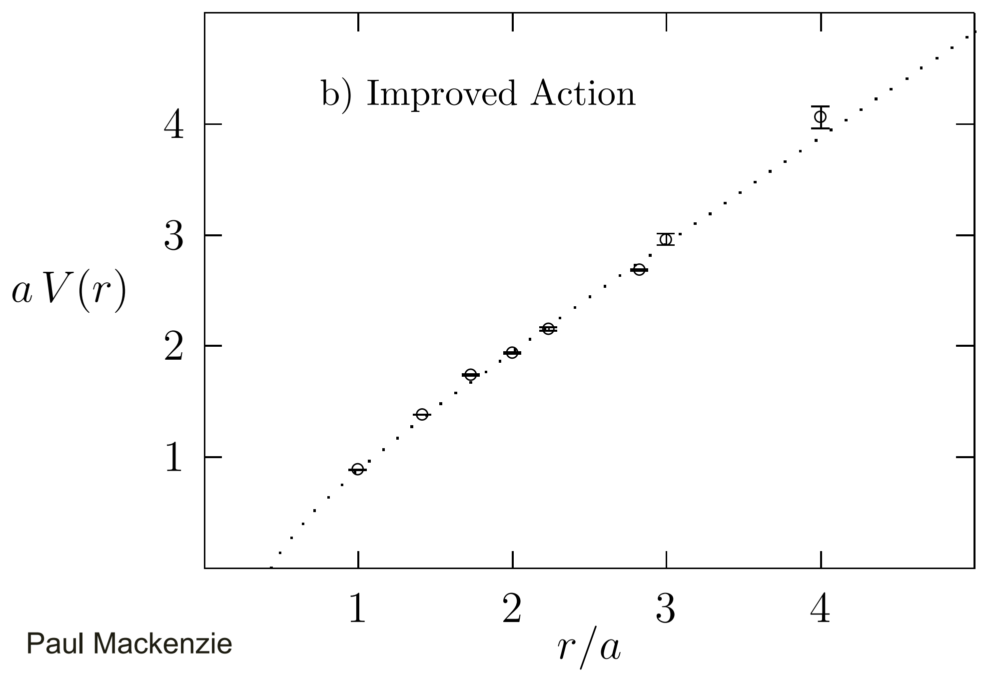
Comparison of Monte Carlo calculation of dozens of different small U loops (points) with perturbation theory (dotted lines).

One-parameter fit in α_s. Shape is a parameter-free prediction of theory.

Verification

Rotation invariance.





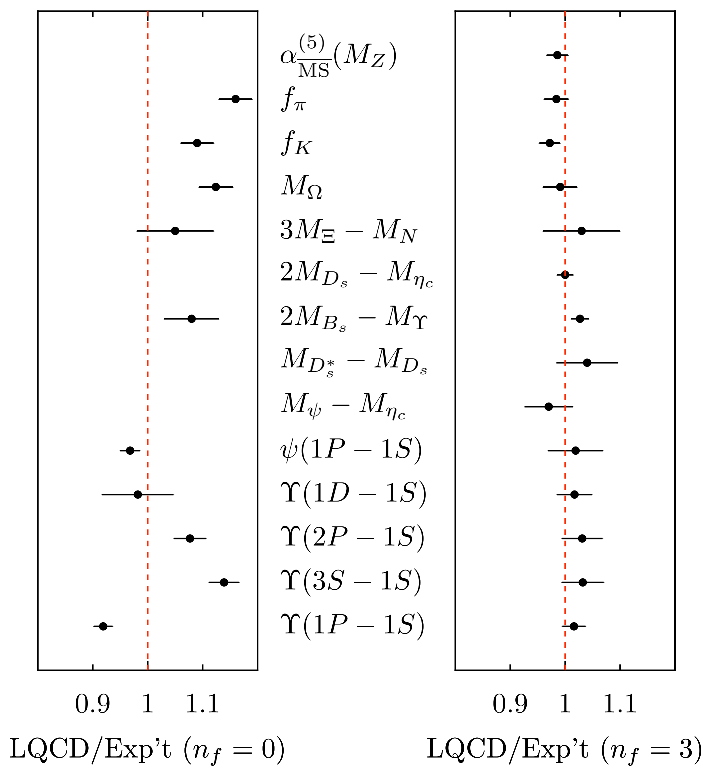
Correctness of a proposed improved action is demonstrated by improved agreement of on-axis and off-axis points of the heavy quark potential.

Alford et al., Phys. Lett. B361:87-94, 1995.

Figure 1: Static-quark potential computed on 6^4 lattices with $a \approx 0.4$ fm using the $\beta = 4.5$ Wilson action and the improved action with $\beta_{\rm pl} = 6.8$.

“Validation”?

The equations of QCD are assumed to be right. Comparison with experiment is a further demonstration that they are being correctly approximated, the icing on the cake of verification.



Post-diction.

Until about ten years ago, fluctuations of quark-antiquark pairs were too expensive to include in simulations, the last uncontrolled approximation.When they were included, 10% disagreements outside error bars, and the simplest quantities agreed with experiment within errors.

Davies et al., Phys. Rev. Lett. 92:022001, 2004.

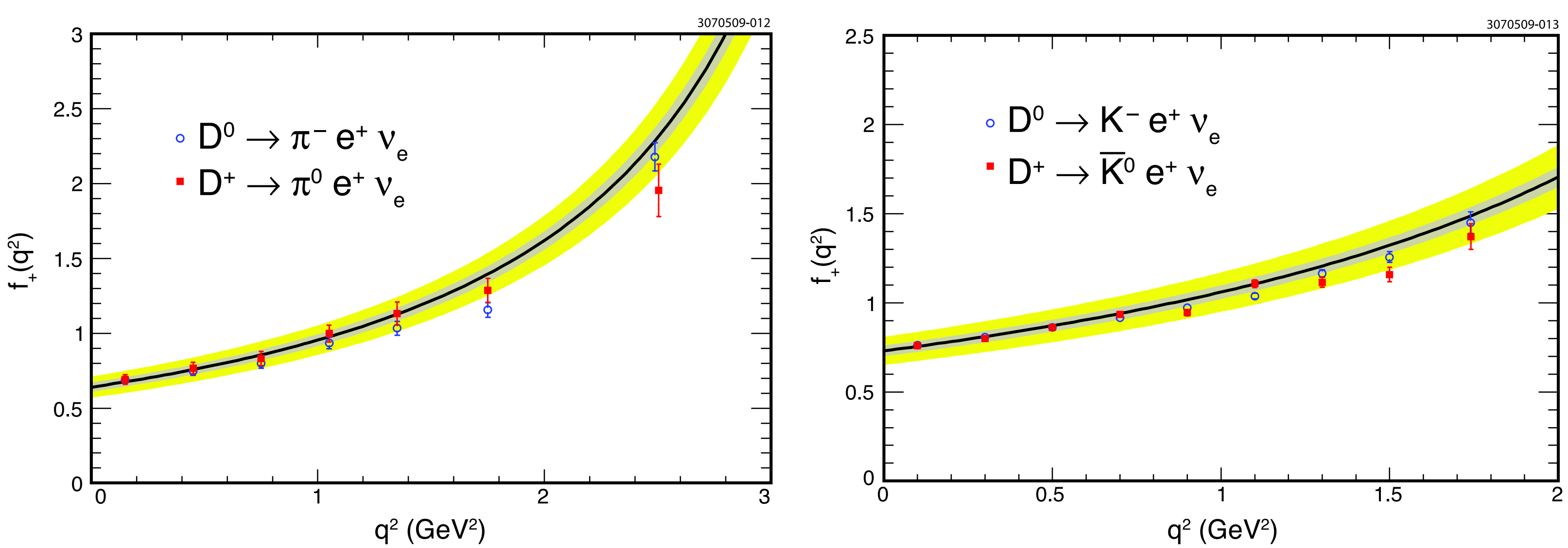


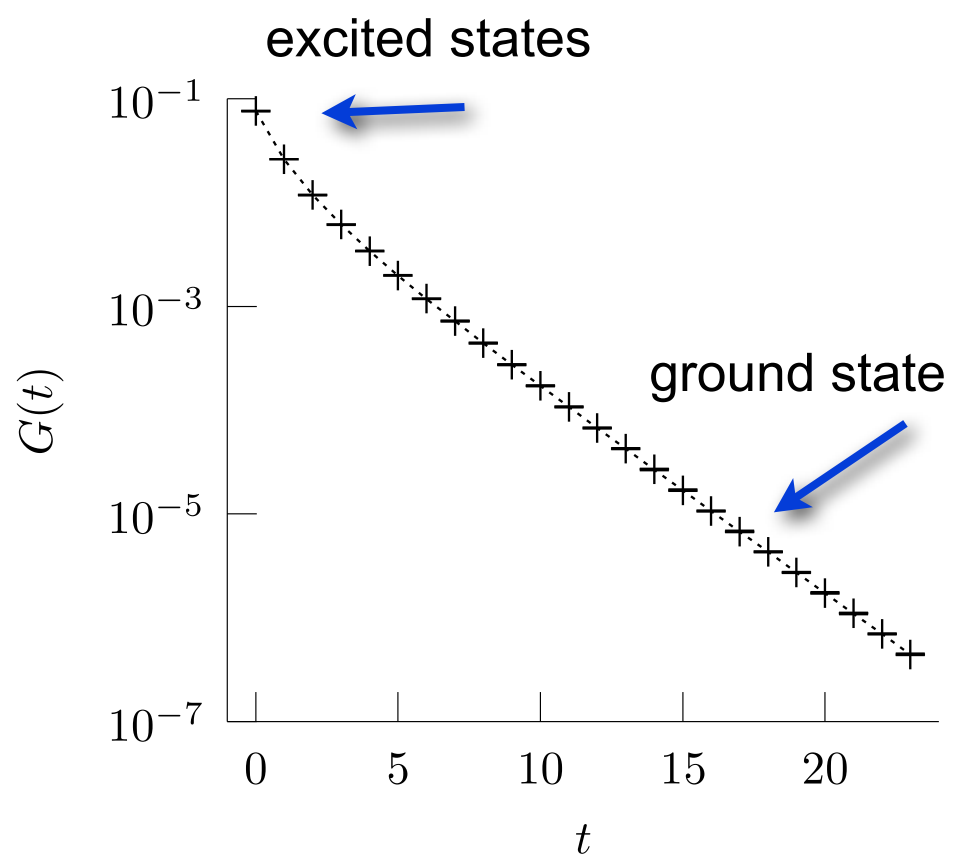
FIG. 8 (color online). $f_+(q^2)$ comparison between isospin conjugate modes and with LQCD calculations [21]. The solid lines represent LQCD fits to the modified pole model [15]. The inner bands show LQCD statistical uncertainties, and the outer bands the sum in quadrature of LQCD statistical and systematic uncertainties.

Prediction.

In 2004, theoretical prediction for shape the D semileptonic form factor was far more precise than experiment. Experimental accuracy has now confirmed and surpassed theory.

CLEO-c, Phys. Rev. **D 80**, 032005 (2009).
Theory graph from Fermilab/MILC, Phys. Rev. Lett. **94**:011601, 2005.

Uncertainty: statistics



Lepage et al., Nucl. Phys. Proc. Suppl. 106:12-20, 2002.

Hadron two-point functions may be obtained by combining quark propagators.
(E.g., $G_\pi(x,y)$=Tr $G(x,y)G(y,x)$.)

On general theoretical grounds, hadrons two-point functions (after Fourier transforming the three spatial dimensions to obtain a momentum eigenstate) are expected to have the form:

$$G_{\rm th}(t; A_n, E_n) = \sum_{n=1}^{\infty} A_n \, {\rm e}^{-E_n t}$$

Parameters may be fit and uncertainties obtained by minimizing χ^2:

$$\chi^2(A_n, E_n) \equiv \sum_{t,t'} \Delta G(t) \; \sigma^{-2}_{t,t'} \, \Delta G(t')$$

$$\Delta G(t) \equiv \overline{G(t)} - G_{\rm th}(t; A_n, E_n)$$

$$\sigma^2_{t,t'} \equiv \overline{G(t)G(t')} - \overline{G(t)} \; \overline{G(t')}$$

Uncertainty: higher order states

Procedure fails when a large number of states are included.

Approximate values expected for energy splittings and amplitudes are known phenomenologically. May be used to estimate effects of higher states by extending χ^2 with priors for expected values of higher states (a Bayesian approach).

$$\chi^2 \quad \rightarrow \quad \chi^2_{\mathrm{aug}} \equiv \chi^2 + \chi^2_{\mathrm{prior}}$$

$$\chi^2(A_n, E_n) \equiv \sum_{t,t'} \Delta G(t)\ \sigma^{-2}_{t,t'}\ \Delta G(t')$$

$$\chi^2_{\mathrm{prior}} \equiv \sum_n \frac{(A_n - \tilde{A}_n)^2}{\tilde{\sigma}^2_{A_n}} + \sum_n \frac{(E_n - \tilde{E}_n)^2}{\tilde{\sigma}^2_{E_n}}$$

Uncertainties in parameters can be estimated from a gaussian approximation to χ^2 around χ_{min}.
Higher order parameters are determined by data when data is accurate enough, or their estimated uncertainty will add to total estimated uncertainty when they are unconstrained.

Uncertainty: discretization

Numerical Analysis $\Rightarrow$

$$\frac{\partial\psi(x_j)}{\partial x} = \Delta_x\psi(x_j) + \mathcal{O}(a^2)$$

$$\frac{\psi(x_j+a)-\psi(x_j-a)}{2a}$$

$$\frac{\partial\psi}{\partial x} = \Delta_x\psi - \frac{a^2}{6}\Delta_x^3\psi + \mathcal{O}(a^4)$$

10–15% for $a = 0.4\,\mathrm{fm}$

1–2% for $a = 0.4\,\mathrm{fm}$

Ignoring gluon interaction, discretization errors may be reduced with next-nearest neighbor interactions as in ordinary numerical analysis.

New wrinkle in quantum field theory: gluon interactions affect one- and two-hop interactions differently. (Different number of *U* matrices at one and two hops.)

Quantum corrections are short-distance, and may be calculated with perturbation theory.

Functional form of un-calculated corrections and expected scale of coefficients are known, a series in powers of *a* and α_s: e.g.,

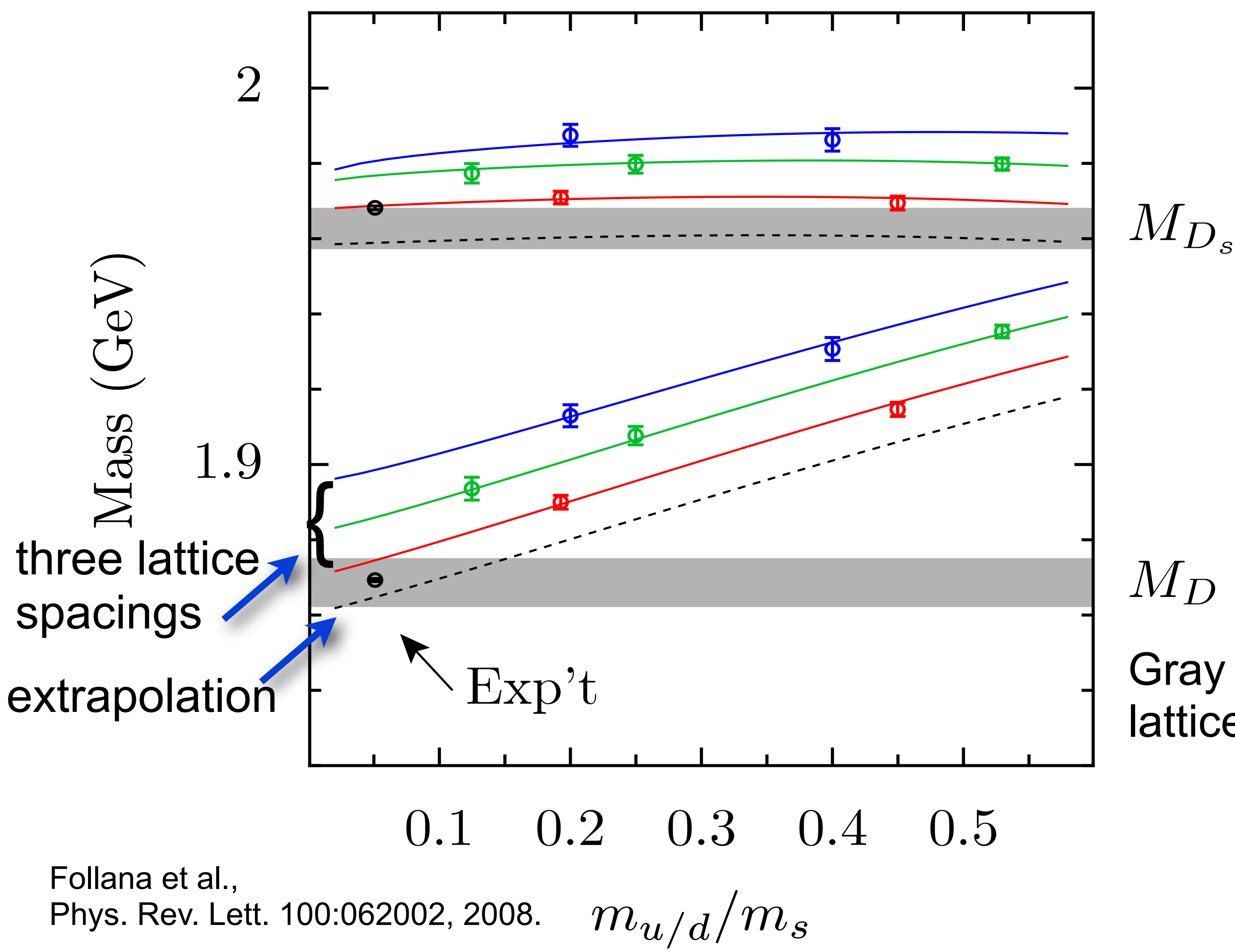
$c_0a^2+c_1a^2\alpha_s+\ldots+d_0a^4+d_1a^4\alpha_s+\ldots$

Effects can be included in continuum extrapolations by adding Bayesian priors to the known functional form of the lattice spacing dependence.

Uncertainty: chiral ($m \to m_{phys}$) extrapolation

For small m, the expected dependence of physical quantities on m can be calculated with chiral perturbation theory, an expansion in the quark mass *m* (or equivalently, in M_π^2) and $m \ln(m)$, valid when M_π and E_π are small compared to the QCD scale.

As with continuum extrapolation, the functional form and expected scale of the coefficients is know, and the effects of undetermined terms can be estimated by including them in Bayesian priors.

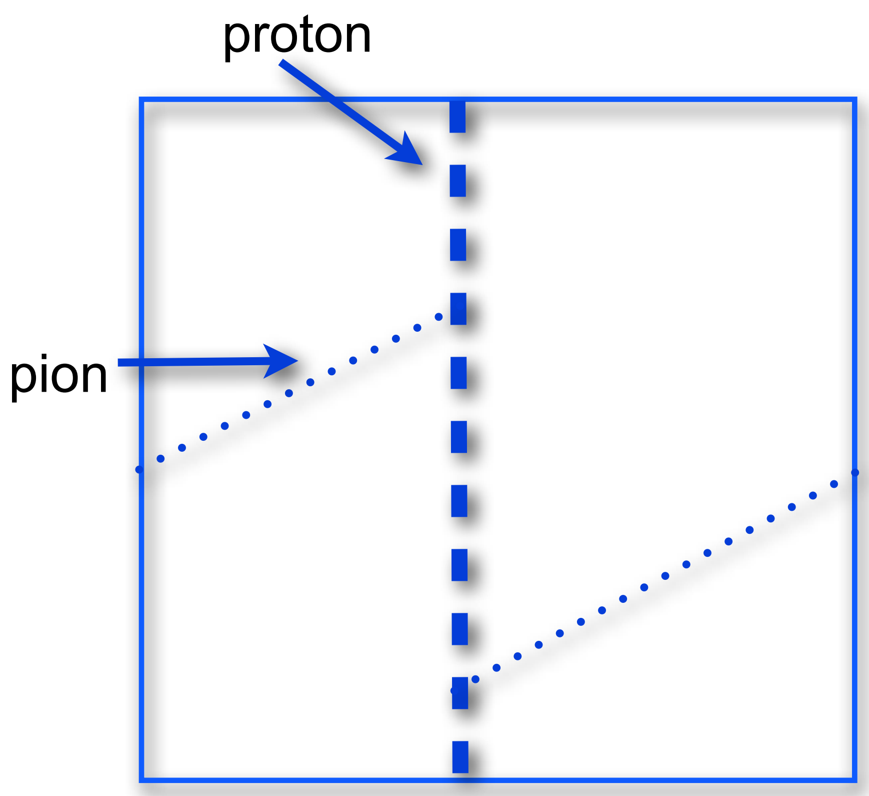


Simultaneous chiral and continuum extrapolations. Bayesian priors included up to order m^3 and $\alpha_s^3 a^2$.

Gray band is final lattice post-diction.

Follana et al.,
Phys. Rev. Lett. 100:062002, 2008.

Uncertainty: finite volume



At large distances, hadron interactions are not sensitive to quark structure. Physics may be approximated by treating protons, pions, etc., as point particles.
With periodic boundary conditions, volume errors are dominated by hadrons emitting a pion (the lightest hadron) that travels out the volume on one side and re-enters on the other.
Effect can be calculated:

$$R_N = \frac{3}{4\pi^2} \sum_{n=1}^{\infty} \frac{m(n)}{\sqrt{n}\lambda_\pi} \left[2\pi \varepsilon_\pi g_{\pi N} e^{-\sqrt{n(1-\varepsilon_\pi^2)}\lambda_\pi} - \int_{-\infty}^{\infty} dy e^{-\sqrt{n(1+y^2)}\lambda_\pi} \tilde{D}^+(y) \right]$$

Exponentially suppressed in the pion mass times the lattice size L.

$$\lambda = M_\pi L$$

Colangelo, Luescher.

Uncertainty can be estimated by calculating the correction, including it, and estimating that the higher order uncertainties are smaller than the included piece.

Example error budget: $B \to D^* l\nu$.

Determines quark mixing matrix element V_{cb}.

Uncertainty	$h_{A_1}(1)$
Statistics	1.4%
$g_{DD^*\pi}$	0.9%
NLO vs NNLO χPT fits	0.9%
Discretization errors	1.5%
Kappa tuning	0.7%
Perturbation theory	0.3%
u_0 tuning	0.4%
Total	2.6%

Bernard et al., Phys. Rev. D79:014506, 2009.

Blue: intrinsic uncertainties of lattice calculations.
Green: removable with improved lattice calculations.
Red: removable by being more careful.

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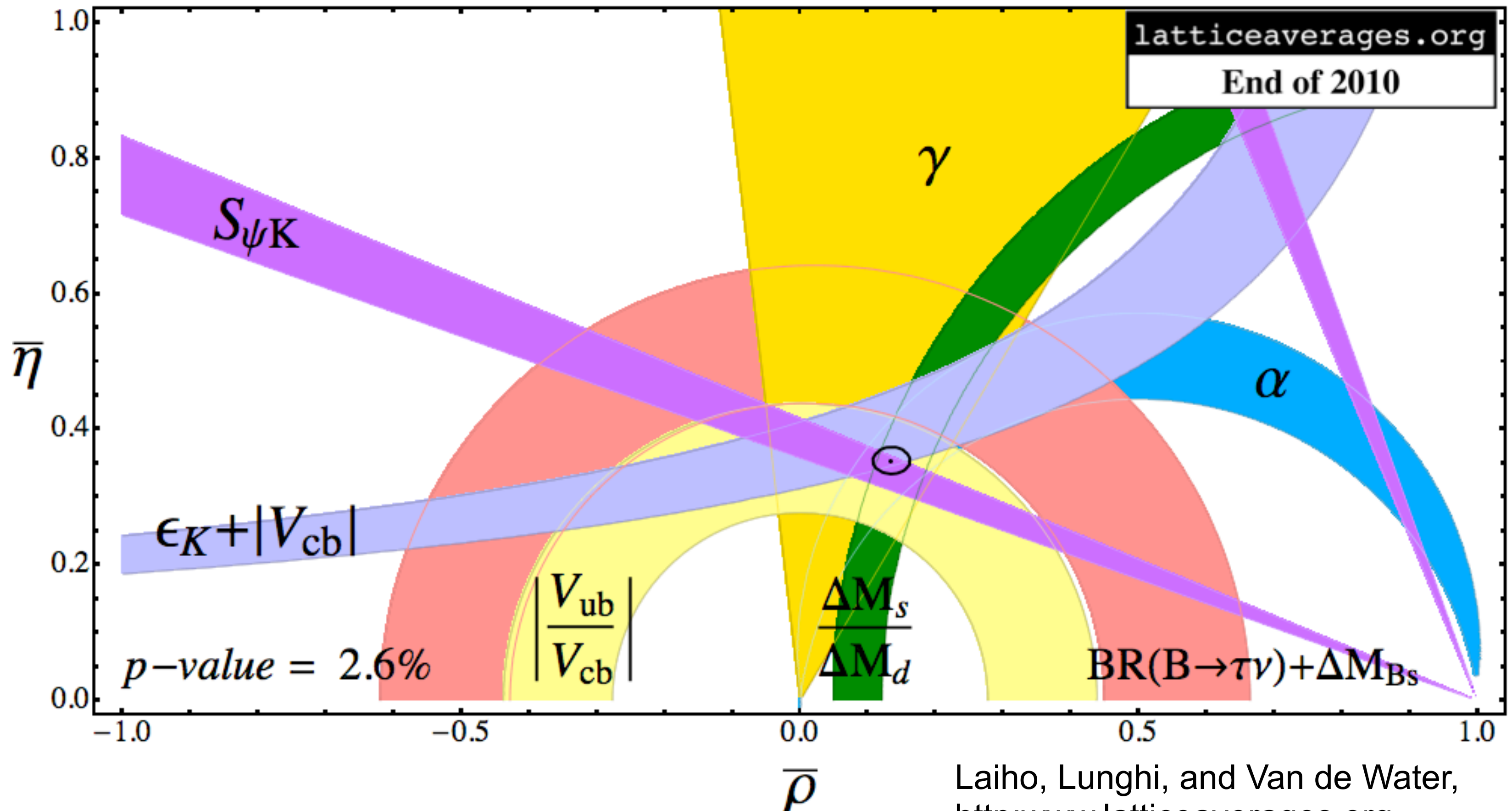
The bottom line: can we see new physics?

There is currently a ~2.5σ discrepancy in determinations of the quark mixing matrix parameters ρ and η from different physical processes.



Laiho, Lunghi, and Van de Water, http:www.latticeaverages.org.

Is this is a signal for new physics? It depends on how bullet proof the uncertainty analysis is in theory and experiment.

Conclusions

- The most important goal of particle physics now is the search for the effects of not-yet-discovered forces and particles.
  - Both directly (as at the LHC) and indirectly (through their effects in the interactions of already discovered particles).
- Some of the most important searches for the effects of new physics on known particles are enabled by lattice gauge theory calculations, and limited by the uncertainty analysis in these lattice calculations.
  - Some experimental measurements are accurate to 0.5%.
  - Precision of the microscope on new physics will become an order of magnitude sharper as lattice QCD uncertainties are pushed from ~5% to 0.5%.
  - Essential to understand the robustness of the uncertainty analysis to decide what the implications are for particle physics.