

Lattice QCD

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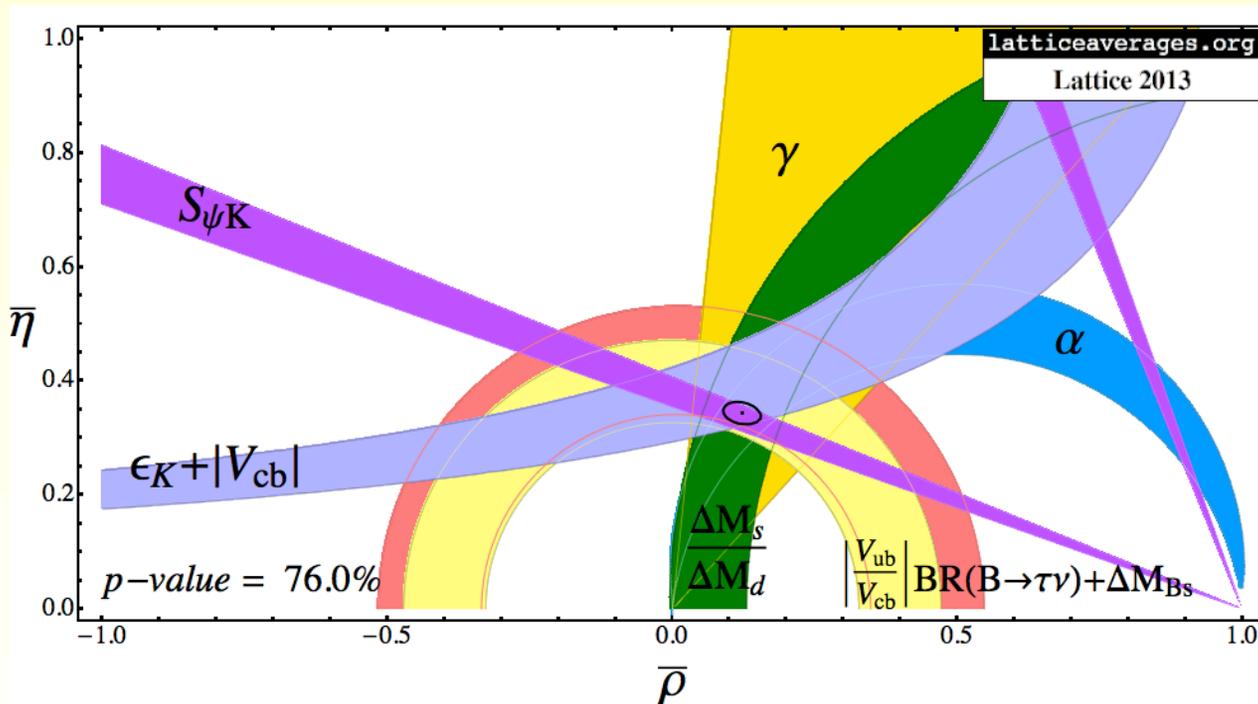
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Why lattice QCD?

Large experimental and theoretical effort dedicated to

- * Searching for **beyond the Standard Model (New Physics)** effects via precise measurements/**SM** predictions of flavour observables.
- * Constraining possible **NP** models.

Laiho, Lunghi, Van de Water PRD81:034503 (2010)



Example: UT fits

$$\text{Experiment} = (\text{known factors}) \times (V_{CKM}) \times \overbrace{(\text{matrix elements})}^{\text{lattice}}$$

Error bands are still dominated by theory errors, in particular due to hadronic matrix elements (encoding **non-perturbative physics**) \rightarrow use **lattice QCD**

Phenomenological goals

Tests of the SM

$$\text{Experiment} = (\text{known factors}) \times (V_{CKM}) \times \underbrace{(\text{matrix elements})}_{\text{lattice}}$$

* Test the SM by overconstraining its parameters.

* Unveil new physics.

Constraining and getting information about beyond the SM theories.

Testing QCD by reproducing the measured spectrum of masses of hadrons.

Precision calculation of SM parameters.

Parameters of the Scalar Sector

* quark masses: m_u, m_d, m_s, m_b, m_c (need $m_{b,c}, \alpha_s$ to test SM)

* elements of the CKM matrix. Higgs couplings)

Hadronic properties: masses, structure, decay constants, form factors for electromagnetic, weak and rare decays, ...

Some points to remember

- # Lattice gauge theories are the same of the theory we are simulating, they are not models. However, we are limited in the things we can calculate efficiently.
- # There are statistical and systematic errors associated with any calculation and one needs to be able to estimate (calculate) them in a rigorous way.
- # Lattice calculations are numerically very intensive.

1.1 Introduction: Path integral formalism

The lattice formulation is based on the **path integral formalism**.

1.1.1 Path integrals in quantum mechanics

(we are going to use $\hbar/(2\pi) = c = 1$)

A simple one-particle 1-d system has $H = p^2/(2m) + V(x)$ with $[x, p] = i$

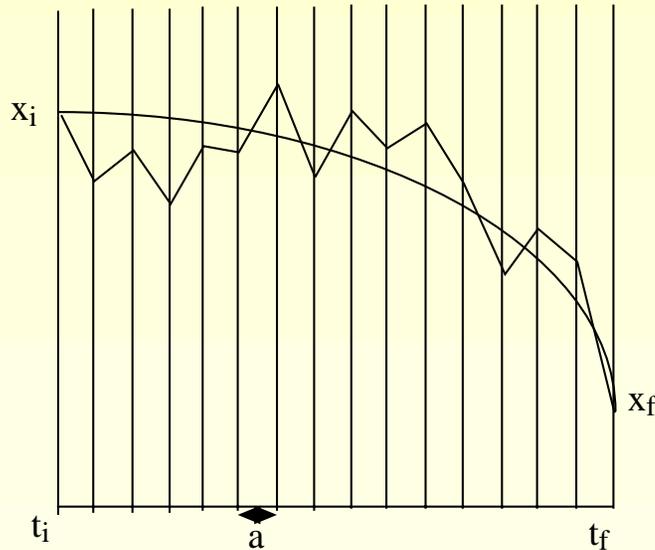
- * Solve Schrödinger equation for simple $V(x)$.
- * Alternatively, calculate the transition amplitude which tells us how a position eigenstate evolves in time. This can be represented by a **path integral**

$$\langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle = \int \mathcal{D}x e^{iS[x]}$$

the integration is over **all possible paths** $x(t)$ with end points x_i and x_f weighted by the exponential of the **action**. The action is defined by

$$S[x] \equiv \int_{t_i}^{t_f} dt L(x, \dot{x}) \equiv \int dt \left[\frac{m\dot{x}(t)^2}{2} - V(x(t)) \right]$$

1.1.1 Path integrals in quantum mechanics



$$\int \mathcal{D}x e^{iS[x]}$$

The classical path is the one for which the action is minimized ($m\ddot{x} = V'$). Path integral allows quantum fluctuations around this.

Discretization of the space: Sum over all possible $x(t)$ can be done by breaking t up into a set of points $t_0 = t_i, t_1, \dots, t_N = t_f$ and integrating over $x_j = x(t_j)$

$$\int \mathcal{D}x(t) = \int dx_1 dx_2 \dots dx_{N-1} \quad \rightarrow \quad N - 1\text{-dimensional integral}$$

* Spacing between t_j points is called a (lattice spacing)

1.1.1 Path integrals in quantum mechanics

Discretization of the action: Evaluate the action at each t_i . For a smooth function $x(t)$:

$$\int_{t_j}^{t_{j+1}} L dt \approx a \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{a} \right)^2 + \frac{1}{2} (V(x_{j+1}) + V(x_j)) \right]$$

$$S[x] = S[x_j; j = 1 \dots N] = \sum_{j=1}^N \int_{t_j}^{t_{j+1}} L dt \approx \sum_{j=1}^N \left[\frac{m}{2a} (x_{j+1} - x_j)^2 + a V(x_j) \right]$$

Goal: develop numerical procedures to evaluate the evolution of the position eigenstate through the path integral (\equiv propagator)

$$\langle x_f | e^{-iH(t_f - t_i)} | x_i \rangle = \int dx_1 dx_2 \dots dx_{N-1} e^{iS[x]}$$

* Phases are hard to handle numerically \rightarrow rotate time to
Euclidean space: $t \rightarrow -it$

1.1.1 Path integrals in quantum mechanics

Knowledge of the propagator as a function of x_f, t_f, x_i, t_i gives complete information about the quantum theory.

In wave function language the propagator can be written as

$$\langle x_f | e^{-H(t_f - t_i)} | x_i \rangle = \sum_n \psi_n^*(x_f) \psi_n(x_i) e^{-E_n(t_f - t_i)} \quad \psi_n(x_i) = \langle E_n | x_i \rangle$$

Example: Take $x_i = x_f = x$ and $T \equiv t_f - t_i$.

$$\langle x | e^{-HT} | x \rangle = \int \mathcal{D}x e^{-S[x]}$$

$$S[x] \equiv \int_0^T L(x, \dot{x}) dt \equiv \int dt \left[\frac{m\dot{x}(t)^2}{2} + V(x(t)) \right]$$

The result is dominated by the ground state $-E_0$ at large T .

$$\langle x | e^{-HT} | x \rangle = \sum_n \psi_n^*(x) \psi_n(x) e^{-E_n T} \xrightarrow{T \rightarrow \infty} |\psi_0(x)|^2 e^{-E_0 T}$$

1.1.1 Path integrals in quantum mechanics

Example: We can generate excited states by inserting x operators at intermediate points and measuring ratios of path integrals

$$\frac{\int \mathcal{D}x x(t_2)x(t_1)e^{-S[x]}}{\int \mathcal{D}x e^{-S[x]}} \xrightarrow{T \rightarrow \infty} |\langle E_0 | x | E_1 \rangle|^2 e^{-(E_1 - E_0)(t_2 - t_1)}$$

* The ground state can not propagate from t_1 to t_2 because x changes parity.

In principle, path integral averages of arbitrary functionals $\Gamma[x]$

$$\langle \langle \Gamma[x] \rangle \rangle = \frac{\int \mathcal{D}x(t) \Gamma[x] e^{-S[x]}}{\int \mathcal{D}x(t) e^{-S[x]}}$$

can be used to compute any physical property of the ground and excited states in the quantum theory.

1.1.2 Evaluation of path integrals: Monte Carlo methods

Evaluation of integrals: **Monte Carlo methods.**

$$\langle\langle\Gamma[x]\rangle\rangle = \frac{\int \mathcal{D}x(t)\Gamma[x]e^{-S[x]}}{\int \mathcal{D}x(t)e^{-S[x]}}$$

that is a weighted average over paths with weight $e^{-S[x]}$.

- * **Configuration:** A particular path described by a vector of numbers $x = x(t_0), x(t_1), \dots, x(t_{N-1})$.
- * **Ensemble:** Set of configurations. We generate a large number N_{conf} of random paths of configurations

$$x^{(\alpha)} \equiv \langle x_0^\alpha, x_1^\alpha, \dots, x_{N-1}^\alpha \rangle \quad \alpha = 1, 2, \dots, N_{conf}$$

in such way that the probability $P[x^{(\alpha)}]$ of obtaining any particular path $x^{(\alpha)}$ is $P[x^{(\alpha)}] \propto e^{-S[x^{(\alpha)}]}$.

1.1.2 Evaluation of path integrals: Monte Carlo methods

Example: Metropolis algorithm (simplest procedure)

- * Start with an initial configuration.
- * $x_i \rightarrow x_i + \xi$ where ξ is a random number in $[-\epsilon, \epsilon]$ (uniform probability distribution).
- * Calculate ΔS for that configuration.
- * Accept the change if $\Delta S < 0$.
- * If $\Delta S > 0$, accept the change if $e^{-\Delta S} > rand(0, 1)$.
- * Repeat for all i and update the configuration.

Correlations: successive paths are highly correlated \rightarrow keep only the configurations generated every N_{cor} - th path.

$$N_{cor} \propto \frac{1}{a^2} \text{ for Metropolis}$$

\Rightarrow Ensemble of configurations with probability e^{-S} .

1.1.2 Evaluation of path integrals: Monte Carlo methods

The weighted average over uniformly distributed paths of any $\Gamma[x]$ is thus given by the Monte Carlo estimator $\bar{\Gamma}$:

$$\langle\langle\Gamma[x]\rangle\rangle = \frac{\int \mathcal{D}x(t)\Gamma[x]e^{-S[x]}}{\int \mathcal{D}x(t)e^{-S[x]}} \approx \bar{\Gamma} \equiv \frac{1}{N_{conf}} \sum_{\alpha=1}^{N_{conf}} (\Gamma[x^{(\alpha)}])$$

And we can estimate statistical errors using

$$\sigma_{\bar{\Gamma}}^2 \approx \frac{1}{N_{conf}} \left\{ \frac{1}{N_{conf}} \sum_{\alpha=1}^{N_{conf}} \Gamma^2[x^{(\alpha)}] - \bar{\Gamma}^2 \right\}$$

statistical errors $\propto 1/\sqrt{N_{conf}}$

1.1.3 Quantum field theory on a lattice: QCD

Lagrangian formulations \rightarrow quantization using paths integrals.

* $x(t) \rightarrow \psi(x)$ or $A_\mu(x)$ with $x = (t, \vec{x})$.

The basic path integral partition function for QCD is

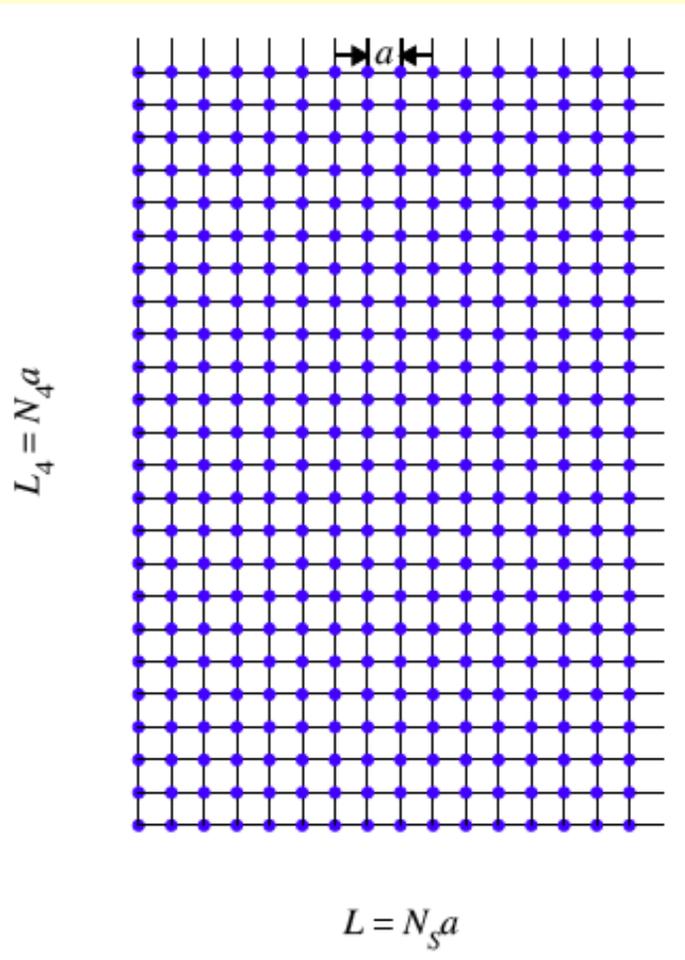
$$\int \mathcal{D}A_\mu \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_{QCD}}$$

with $S_{QCD} = \int dx^4 \mathcal{L}_{QCD}$ and

$$\mathcal{L}_{QCD} = \frac{1}{2} \text{Tr} F_{\mu\nu}^2 + \bar{\psi}(\gamma \cdot D + m)\psi = \frac{1}{2} \text{Tr} F_{\mu\nu}^2 + \bar{\psi} M[A]\psi$$

g is the bare QCD coupling ($\alpha_s = g^2/4\pi$), D is the covariant derivative, $(\partial_\mu - igA_\mu)$, and F is field strength $(\partial_\mu A_\nu - \partial_\nu A_\mu + ig[A_\mu, A_\nu])$

1.1.3 Quantum field theory on a lattice: QCD



- * Take 4-d box (Eucl.) space-time
- * Discretize the QCD action in the lattice

$$(t, \vec{x}) \Rightarrow \vec{n} = (n_t a, n_x a, n_y a, n_z a)$$

$$\psi(x) \rightarrow \psi_n$$

with $n_t = 1, \dots, N_t$ and $n_i = 1 \dots N_s$.

$$\rightarrow \int d^4x \Rightarrow a^4 \sum_{n_i}, \quad \dim(M) = 4 \cdot 3 \cdot (N_s^3 \cdot N_4)$$

- * Replace derivatives by finite differences

$$\partial_\mu f(x) \rightarrow \frac{f(x + a\hat{\mu}) - f(x - a\hat{\mu})}{2a}$$

→ Path integral becomes a product of integrals over each of the fields

$$\int \mathcal{D}\psi \mathcal{D}\bar{\psi} \rightarrow \prod_n \int d\psi_n d\bar{\psi}_n$$

Lattice acts as an UV cut-off ($p_i > \pi/a$ are not allowed)

1.2 Lattice QCD: Discretization of gluon fields

Key feature: **gauge invariance** (even at finite a).

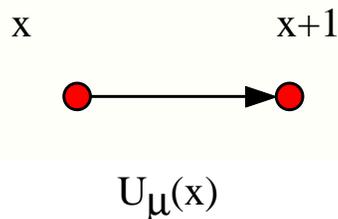
* It is impossible to formulate a discretized version of QCD in terms of A_μ and gauge invariant.

* Instead of specifying gauge field by values at the sites, use variables on the links joining the sites \implies **gluon fields live on links while quark fields live on sites.**
 (gluon fields transport colour from one place to another)

** Classically the **link variable** joining sites x and $x + a\hat{\mu}$ is

$$U_\mu(x) \equiv \mathcal{P}exp \left(-i \int_x^{x+a\hat{\mu}} gA \cdot dy \right)$$

** So I have $A_\mu \equiv A_\mu^b T_b$ \rightarrow $U_\mu = e^{-iagA_\mu}$
 continuum lattice

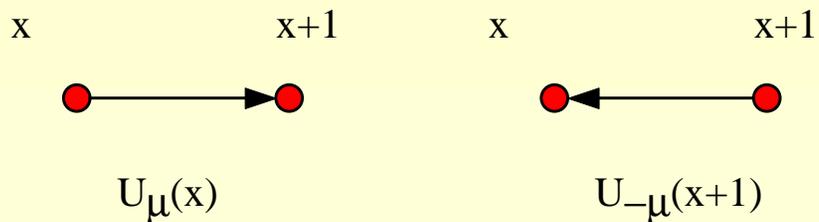


$$U_\mu^{(g)}(x) = G(x)U_\mu(x)G^\dagger(x + a_\mu)$$

$$\psi^{(g)}(x) = G(x)\psi(x)$$

$G(x)$ is a gauge (3×3 colour matrix) transformation

1.2. Lattice QCD: Discretization of gluon fields



* $U_\mu(x)$ are 3×3 unitary matrices

$$UU^\dagger = 1 \rightarrow$$

$$U_{-\mu}(x+a) = U_\mu^{-1} = U_\mu^\dagger(x)$$

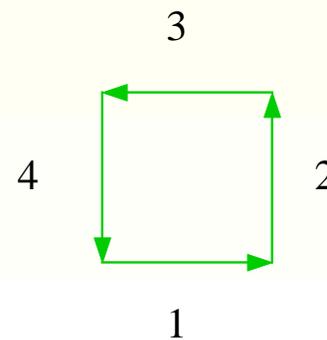
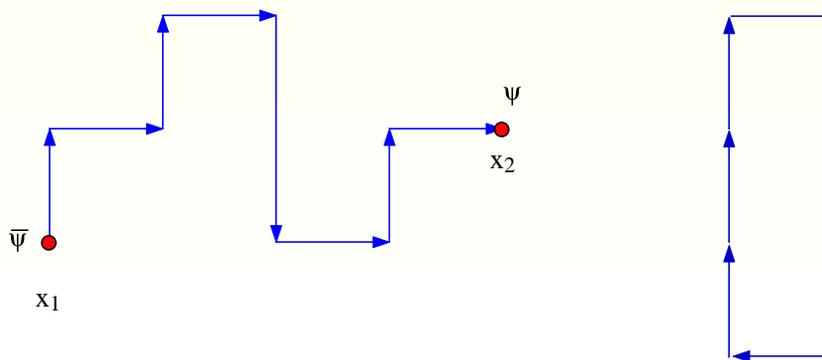
I need to build gauge-invariant objects (remember, $G^\dagger G = 1$).

* Gauge invariant derivatives: $\Delta_\mu f(x) \equiv \frac{1}{a} [U_\mu(x)f(x+a\hat{\mu}) - f(x)]$

* Open strings with quarks at ends

$$\bar{\psi}(x_2) \text{string}(x_1, x_2) \psi(x_1)$$

* Closed strings of U 's



1.2. Lattice QCD: Discretization of gluon fields

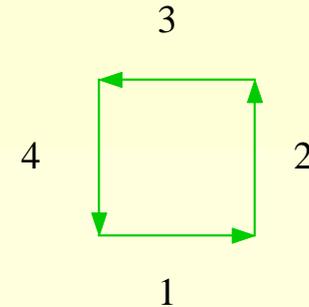
Wilson glue action: Simplest

discretization of

$$S_g^{QCD} = \int d^4x \frac{1}{4g^2} \text{Tr} F_{\mu\nu} F^{\mu\nu} \text{ is.}$$

$$S = \frac{6}{g^2} \sum_p \left[1 - \frac{1}{3} \text{ReTr}(U_p) \right]$$

* 1×1 gluon loop (plaquette)



$$U_p = (U_1)_{ij} (U_2)_{jk} (U_3)_{kl} (U_4)_{li} = U_i(x) U_j(x + \hat{i}) U_i^\dagger(x + \hat{j}) U_j^\dagger(x)$$

* Wilson glue action is conventionally written

$$S_{g,QCD} = \beta \sum_p \left(1 - \frac{1}{N_c} \text{ReTr} U_p \right); \quad \beta \equiv \frac{2N_c}{g^2}$$

* It has $\mathcal{O}(a^2)$ errors.

a is not explicit in the action (it is the only parameter of the pure gluon theory). We only know a after the calculation.

* The value of $a(\equiv \Lambda_{QCD})$ depends on $\beta(\equiv \text{bare } \alpha_s)$.

1.2. Lattice QCD: Discretization of gluon fields

Exercise: For a simple $U(1)$ gauge transformation, $e^{i\alpha(x)}$, show that

$$\begin{aligned}U_{\mu}^{(g)}(x) &= G(x)U_{\mu}(x)G^{\dagger}(x+a_{\mu}) \\ \psi^{(g)}(x) &= G(x)\psi(x) \\ \bar{\psi}^{(g)}(x) &= \bar{\psi}(x)G^{\dagger}(x)\end{aligned}$$

is equivalent to the QED-like gauge transformation in the continuum
 $A_{\mu}^{(g)} = A_{\mu} - \partial_{\mu}\alpha$.

1.2. Lattice QCD: Discretization of gluon fields

Exercise: Probe that the Wilson action

$$S_{g,QCD} = \beta \sum_p \left(1 - \frac{1}{N_c} \text{ReTr}U_p\right); \quad \beta = \frac{2N_c}{g^2}$$

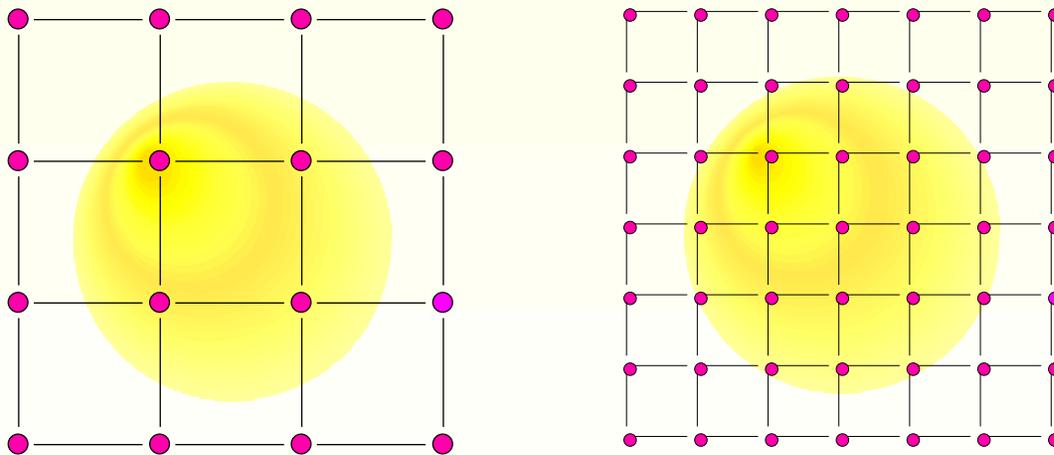
reduces to the continuum gluon action up to $\mathcal{O}(a^2)$ corrections.

1.2.1 Improvement of the lattice actions

Key point to get high precision results

Discretization errors ($a \neq 0$): Obvious source of systematic errors

- * For a fixed L cost of lattice calculations grows as $1/a^4$
- * Other factors that increase the calculation cost with $1/a$
 - ** Physical sizes (eg. of glueball) grow in lattice units as a decreases.
 - ** Decorrelation time to new configurations on physical scale grows as $1/a^2$



1.2.1 Improvement of the lattice actions

Discretization errors ($a \neq 0$): Obvious source of systematic errors

$$\text{cost}(\text{lattice QCD}) \approx \left(\frac{L}{a}\right)^4 \frac{1}{a} \frac{1}{m_\pi^2 a}$$

a small increases N and cost \rightarrow **improve the discretization** instead

* Discretization of derivatives:

$$\left. \frac{\partial^2 \psi(x_j)}{\partial x^2} \right|_{cont} = \Delta_x \psi(x_j) |_{lat}.$$

$$\text{up to } \mathcal{O}(a^2) : \Delta_x \psi(x_j) |_{lat} = \Delta_x^{(2)} \psi(x_j + a) + \mathcal{O}(a^2) = \frac{\psi(x_j + a) - 2\psi(x_j) + \psi(x_j - a)}{a^2}$$

$$\text{up to } \mathcal{O}(a^4) : \Delta_x \psi(x_j) |_{lat} = \Delta_x^{(4)} \psi(x_j) = \Delta_x^{(2)} \psi(x_j) - \frac{a^2}{12} (\Delta_x^{(2)})^2 \psi(x_j) + \mathcal{O}(a^4)$$

1.2.1 Improvement of the lattice actions

Improving the gluon action

Errors in Wilson plaquette action are $\mathcal{O}(a^2)$: $\approx 4\%$ at $a = 0.1 \text{ fm}$.

\implies (Symanzik) improved the action to reduce the errors at fixed a .

* Improvement terms: bigger loops (2×1 rectangles)

$$S_{g,QCD} = \frac{\beta}{N_c} \sum (N_c - \frac{5c_1}{3} \text{ReTr}U_p + \frac{c_2}{12} \text{ReTr}(U_{2 \times 1} + U_{1 \times 2}))$$

** Coefficients chosen to cancel a^2 . However, in QCD, they get renormalized by radiative corrections

$$c_i = 1 + c_i^{(1)} \alpha_s + \dots$$

- Need to match continuum QCD which has gluons with momentum $> \pi/a \rightarrow$ **perturbative** calculation of c_i

\rightarrow After including LO radiative corrections, left with $\mathcal{O}(1)\alpha_s a^2$ errors ($\approx 1\%$ at $a = 0.1 \text{ fm}$).

1.3 Lattice QCD: Discretization of the fermionic action

Big challenge of lattice QCD: QUARKS

$$S_{QCD} = S_G[A] + \sum_x \bar{\psi}(\gamma \cdot D + m)\psi = S_G[A] + \bar{\psi}M[A]\psi$$

Quarks fields anticommute: can not be represented by ordinary numbers in a computer

→ Do quark functional integral analytically by hand

$$\begin{aligned} Z &\equiv \int \mathcal{D}A_\mu \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_{QCD}} = \int \mathcal{D}A_\mu e^{-S_G[A]} \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\bar{\psi}M[A]\psi} \\ &= \int \mathcal{D}A_\mu \det(M[A]) e^{-S_G[A]} = \int \mathcal{D}A_\mu e^{-S_{eff}[A]} \\ \langle 0 | \mathcal{O}[\bar{\psi}, \psi, A] | 0 \rangle &= \frac{1}{Z} \int \mathcal{D}A_\mu F[M^{-1}, A] e^{-S_{eff}[A]} \end{aligned}$$

⇒ $S_{eff}[A] = S_G + \ln \det(M[A])$: fermionic determinant (one per flavour)

Problem reduced to an integration over background gluon configurations.

1.3.1 Lattice QCD: Calculation of expected values

Generate an ensemble of configurations U distributed according to $e^{-S_{eff}}$ and calculate the ensemble average of O

$$\langle 0|O|0\rangle = \langle\langle O \rangle\rangle = \frac{1}{N_{conf}} \sum_{i_{conf}=1}^{N_{conf}} O_{i_{conf}}$$

* Statistical errors $\propto 1/\sqrt{N_{conf}}$: Typically need N_{conf} = many hundreds

1.3.1 Lattice QCD: Calculation of expected values

Example: hadron mass Choose an operator that creates the hadron at time 0 and destroys it at T

* Any operators with correct J^{PC} will do.

$$\frac{1}{Z} \langle 0 | H^\dagger(T) H(0) | 0 \rangle = \frac{\int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} (\sum_{\vec{x}} \bar{\psi}^a \Gamma \psi^b(\vec{x}))_T (\bar{\psi}^b \Gamma \psi^a)_0 e^{-S_{QCD}}}{\int \mathcal{D}U \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_{QCD}}}$$

and, after integration over quark fields ($a \neq b$)

$$\begin{aligned} \frac{1}{Z} \langle 0 | H^\dagger(T) H(0) | 0 \rangle &= \frac{\int \mathcal{D}U \text{Tr}_{\text{spin,color},\vec{x}} (M_a^{-1} \Gamma M_b^{-1} \Gamma) \det M e^{-S_G}}{\int \mathcal{D}U \det M e^{-S_G}} \\ &= \frac{\int \mathcal{D}U \text{Tr}_{\text{spin,color},\vec{x}} (M_a^{-1} \Gamma M_b^{-1} \Gamma) e^{-S_{eff}}}{\int \mathcal{D}U e^{-S_{eff}}} \end{aligned}$$

Calculate this by averaging the $\text{Tr} M^{-1}$ factors over sets of configurations distributed according to $e^{-S_{eff}}$

1.4.1 Lattice QCD: Calculation of expected values

$$\frac{1}{Z} \langle 0 | H^\dagger(T) H(0) | 0 \rangle = \frac{\int \mathcal{D}U \text{Tr}_{\text{spin,color},\tilde{x}} (M_a^{-1} \Gamma M_b^{-1} \Gamma) e^{-S_{eff}}}{\int \mathcal{D}U e^{-S_{eff}}}$$

The lhs of previous expression is related to the hadron mass as

$$\frac{1}{Z} \langle 0 | H^\dagger(T) H(0) | 0 \rangle = \sum_n |\langle 0 | H | n \rangle|^2 e^{-m_n T} \xrightarrow[T \rightarrow \infty]{} |\langle 0 | H | 0 \rangle|^2 e^{-m_0 T}$$

where n is the n th state with quantum numbers set by Γ .

Improve convergence: smearing H with a wavefunction

$$H = \bar{\psi}(\vec{x}_2) \Gamma \phi(|\vec{x}_2 - \vec{x}_1|) \psi(\vec{x}_1) \rightarrow \text{better overlap with } n = 0.$$

* Make several different H to extract excited states.

1.4.2 Quenched approximation

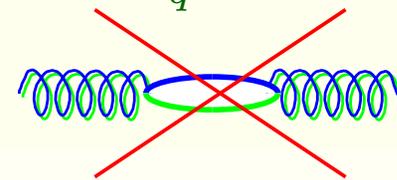
$$\frac{1}{Z} \langle 0 | H^\dagger(T) H(0) | 0 \rangle = \frac{\int \mathcal{D}U \text{Tr}_{\text{spin,color},\tilde{x}} (M_a^{-1} \Gamma M_b^{-1} \Gamma) e^{-S_G + \ln(\det M)}}{\int \mathcal{D}U e^{-S_G + \ln(\det M)}}$$

* **Valence quarks** (quarks in the operator): need to calculate M^{-1} to integrate quarks out

** Very costly $\propto \frac{1}{am_q}$ \rightarrow simulate unphysical (larger) masses

* **Sea quarks** ($q\bar{q}$ pairs in vacuum): need to include $\det(M)$ in making gluon configurations \rightarrow very expensive to include in simulations, especially for light quarks $m_q \rightarrow 0$

Quenched approximation



Not including $\det(M) \equiv$ cutting out quark-antiquark pair production

** Important sea quarks: u, d, s ($N_f = 2 + 1$ simulations). Effect of c starting to be included ($N_f = 2 + 1 + 1$). b, t have not effect.

1.4.3. Discretization of light quarks

Simplest discretization: Naive quarks

$$S_q = \sum_x \bar{\psi}(x)(\gamma \cdot \Delta + ma)\psi(x)$$

$$\Delta_\mu \psi(x) \equiv \frac{1}{2a_0} (U_\mu(x)\psi(x + \hat{\mu}) - U_\mu^\dagger(x - \hat{\mu})\psi(x - \hat{\mu}))$$

* Advantages:

** Discretization errors $\mathcal{O}(a^2)$

** Exact chiral symmetry ($\psi \rightarrow e^{i\alpha\gamma_5}\psi$) \rightarrow important properties

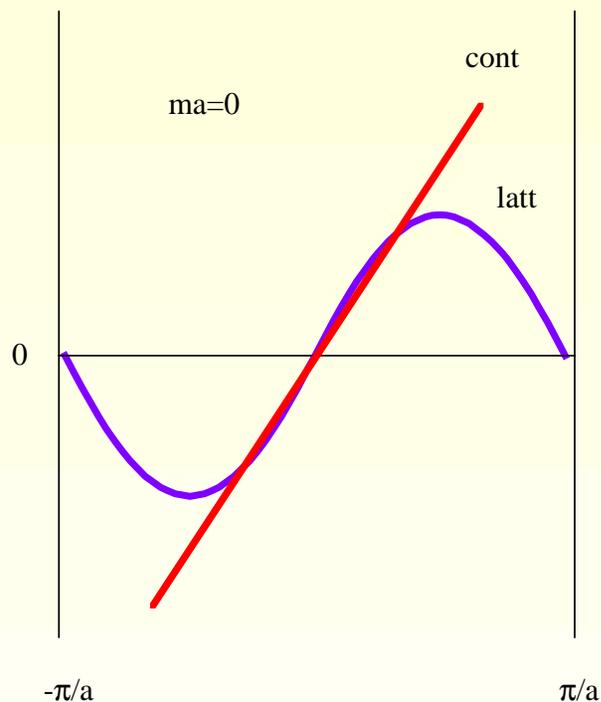
$$m_\pi \xrightarrow{m_u/d \rightarrow 0} 0$$

** Eigenvalue spectrum of M similar to continuum

1.4.3. Discretization of light quarks

* Disadvantages: **Doubling problem.**

Continuum inverse quark propagator (1 zero when $m \rightarrow 0$)



$$G^{-1}(p) = i\gamma_{\mu}p_{\mu} + m$$

On the lattice (16 zero when $m \rightarrow 0$)

$$G^{-1}(p) = i\gamma_{\mu} \frac{\sin p_{\mu}a}{a} + m$$

Similar behaviour to continuum
at $p \approx -\pi$ and $p \approx \pi$!

→ There are 2^d quarks in d
dimensions instead of only 1.

doublers: 15 (for $\text{dim}=4$) unphysical extra states.

1.4.3. Discretization of light quarks

Different ways of discretizing the fermionic action, although they must be identical in the continuum limit, have different properties.

- * Approach to the **doubling problem**.
- * Chiral (and other) symmetries.
- * Simulation cost.
- * Discretization errors.

Wilson, clover, twisted mass, Ginsparg-Wilson (Neuberger, domain wall, fixed-point), staggered, ...

Key ingredient: Highly improved actions

→ same errors with larger a

All must agree in the continuum limit

1.4.4. Discretization of heavy quarks

- # Problem is discretization errors ($\simeq m_Q a, (m_Q a)^2, \dots$) if $m_Q a$ is large.
- * **Effective theories:** Need to include multiple operators matched to full QCD **B-physics** ✓
- ** HQET (static,...): systematic expansion in $1/m_h$.
- ** NRQCD: systematic (non-relativistic) expansion in (v_h/c) .
- ** Fermilab, RHQ, ...
- * **Relativistic (improved) formulations:**
 - ** Allow accurate results for **charm** (especially twisted mass, HISQ (Highly improved staggered quarks)).
 - ** Advantages of having the same formulation for light and heavy: ratios light/heavy, PCAC for heavy-light, ... Also simpler tuning of masses.
 - ** Also for **bottom**: Results for $m_c \dots \leq m_b$ and extrapolation to m_b (twisted mass, HISQ).

2. Physical results: Tests of Lattice QCD

2.1. Steps of a typical lattice calculation

* Choice of parameters: Volume (lattice spatial and temporal size), lattice spacing through bare QCD coupling constant (determined **after** the calculation is completed).

Typical lattice spacing $a \sim 0.1 \text{ fm}$ or $1/a \sim 2\text{GeV}$

$m_\pi L \sim 2.5 - 5$ (need $m_\pi L \geq 4$ to control FV errors at 1%)

* Choice of gluon and quark formulations and number of quarks flavours and masses in lattice units (physical masses determined **after** the calculation is completed).

Unquenched calculations with realistic vacuum polarization effects

** $N_f = 2$ $m_u = m_d$ and no sea strange quarks.

** $N_f = 2 + 1$ $m_u = m_d$ plus a heavier sea strange quark (usually close to/or the physical value).

** $N_f = 2 + 1 + 1$ Add sea charm quarks too (just starting).

** Partially quenched: Unquenched calculation with $m_{sea} \neq m_{val.}$

** Full QCD: Unquenched calculation with $m_{sea} = m_{valence}$.

2.1. Steps of a typical lattice calculation

* Generation of ensembles of gluon configurations using importance sampling with $e^{-S_{eff}}$.

* Invert quark matrix \rightarrow quark propagators on each gluon configuration.

$$\begin{aligned} & \int [\mathcal{D}\psi][\mathcal{D}\bar{\psi}][\mathcal{D}A] \bar{\psi}(x)^{f1,a} \psi(x)^{f2,a} \bar{\psi}(y)^{f2,b} \psi(y)^{f1,b} e^{-S_{QCD}} \\ &= \int [\mathcal{D}A] \left(M_{x,y}^{-1,f1}[A] \right)^{ab} \left(M_{y,x}^{-1,f2}[A] \right)^{ba} \det(M) e^{-S_{QCD}} \end{aligned}$$

* Calculate correlators (putting together quark propagators and/or gluon fields)

* Average over configurations \rightarrow get statistical errors.

* Fit correlators to their expected theoretical form \rightarrow extract physical quantities (hadron masses, matrix elements ...)

$$\frac{1}{Z} \langle 0 | H^\dagger(T) H(0) | 0 \rangle = \sum_n |\langle 0 | H | n \rangle|^2 e^{-m_n T} \xrightarrow{T \rightarrow \infty} |\langle 0 | H | 0 \rangle|^2 e^{-m_0 T}$$

excited states from subleading exponentials \rightarrow have a much weaker statistical signal.

2.1. Steps of a typical lattice calculation

* **Determining the 5 parameters of the lattice action:** lattice spacing a and quark masses.

** Need experimental input to determine lattice spacing a in GeV : $2S - 1S$ splitting in Υ system, m_N , m_Ω , m_Ξ , f_π , the quark potential $(r_0, r_1), \dots$

→ this also determines α_s .

** Use experimentally measured hadron masses as inputs to fix m_u, m_d, m_s, m_c, m_b , for example: $m_\pi, m_K, m_{D_s}, m_{B_s}$.

* Repeat the process at **several** values of a and quark masses: check a errors are under control.

* Extrapolate to the continuum limit ($a \rightarrow 0$), to the physical quark masses (CHPT) and infinite volume limit.

* Calculate (estimate) systematic errors.

2.2 Error analysis

In order to have **precision calculations** (few % errors) we need unquenching and estimate all possible sources of errors.

* **Statistical errors**: From Monte Carlo integration. Also need to include errors in the fitting procedure to extract physical quantities from correlation functions.

$$\text{statistical errors} \propto 1/\sqrt{N_{conf}}$$

* **Finite lattice spacing**: we need simulations at different values of a , to extrapolate to the continuum limit $a \rightarrow 0$.

To simulate at small values of a while keeping the physical L constant is very expensive

→ **Improved actions** (and operators) decrease the error, making the extrapolation from a given set of lattice spacings more precise.

* Typically, $errors \propto a, a^2, \alpha_s a^2$

* Estimates by power counting and/or comparison of results at the lowest values of a .

2.2 Error analysis

- * **Renormalization constants:** The lattice is an ultraviolet regulator. We need to calculate renormalization constants to relate quantities calculated in the lattice with quantities calculated in a different scheme.

$$\langle \mathcal{O}^{cont} \rangle = Z^{lat} \langle \mathcal{O}^{lat} \rangle$$

- ** Lattice perturbation theory: perturbative errors.

$$Z = z^0 + z^1 \alpha_s + z^2 \alpha_s^2 + \mathcal{O}(\alpha_s^3)$$

- ** Nonperturbative methods: syst.+stat. errors

Impose that suitable **Green functions**, computed between external off-shell quark and gluon states in a fixed gauge coincide with their tree level value

$$Z_{\mathcal{O}}(\mu a, g(a)) \langle p | \mathcal{O} | p \rangle |_{p^2 = -\mu^2} = \langle p | \mathcal{O} | p \rangle_0 \quad \text{with } \mathcal{O} = \bar{\psi} \Gamma \psi$$

2.2. Error analysis

* **Chiral extrapolations:** In practise, most of the times we are not able to simulate at physical values of the light quark masses $m_{u,d}$. Usually no problems to get m_s right.

→ needs to extrapolate to the physical light masses

use Chiral Perturbation Theory (CHPT).

** Need simulations for several values of $m_{u,d}$.

** Simulated masses need to be small enough ($m_{u,d} \leq m_s/2$).

Chiral Perturbation Theory

- It is the effective theory that describe QCD at low energies. **It is not a model!**
- Based on the concept of effective field theory.
 - * Quantum field theory described by the most general lagrangian where operators are built with the relevant degrees of freedom at those energies, and it is compatible with all the symmetries of the original theory.

Chiral Perturbation Theory

Information about the heavier degrees of freedom (high energy physics) is contained in the couplings modulating the operators c_{2n}^i .

$$\mathcal{L}^{CHPT}(U, D^\mu U) = \sum_n \sum_i c_{2n}^i \mathcal{L}_{2n}^i(U, D^\mu U)$$

- Formulated in terms of the relevant degrees of freedom at low energies ($< 1\text{GeV}$): π , K and η (collected in the unitary 3×3 matrix U)
- Organized in powers of these light masses and external momentum (\equiv derivatives).
- Keep the symmetries (chiral symmetry) of QCD.

Chiral Perturbation Theory

- On the lattice: Look to a typical expression for hadron masses and decay constants at NLO.

$$M_{P_{xy}} = \mu(m_x + m_y) \left\{ \frac{1}{16\pi^2 f^2} \left(F_1(l(m_{ab}^2)) + a^2 F_2(l(m_{ab}^2)) \right) + \frac{\mu}{f^2} F_3^{valence}(L_i)(m_x + m_y) + \frac{\mu}{f^2} F_3^{sea}(L_i)(m_u + m_d + m_s) + C a^2 + \text{analytic NNLO} \right\}$$

$$f_{P_{xy}} = f \left\{ 1 + \frac{1}{16\pi^2 f^2} \left(F'_1(l(m_{ab}^2)) + a^2 F'_2(l(m_{ab}^2)) \right) + \frac{\mu}{f^2} F'_3{}^{valence}(L_i)(m_x + m_y) + \frac{\mu}{f^2} F'_3{}^{sea}(L_i)(m_u + m_d + m_s) + C' a^2 + \text{analytic NNLO} \right\}$$

with $l(m^2) \equiv m^2 \ln \frac{m^2}{\Lambda^2}$ and $m_{ab}^2 = \mu(m_a + m_b) + a^2 \Delta_{ab}$. L_i are the couplings of the p^4 CHPT lagrangian.

2.2. Error analysis

* **Finite volume:** keep $m_\pi L > 4$. Estimate errors by

** Repeat the calculation for a fixed a and quark masses for several volumes.

** Use **CHPT**: Fit data with finite volume expressions and extrapolate to infinite volume:

$$m^2 \left(\ln \frac{m^2}{\Lambda^2} + \frac{4}{mL} \sum_{\vec{r} \neq 0} \frac{K_1(|\vec{r}|mL)}{|\vec{r}|} \right) \quad \xrightarrow{\text{finite volume}} \quad \text{infinite volume} \quad l(m^2) \equiv m^2 \left(\ln \frac{m^2}{\Lambda^2} \right)$$

L is the spatial dimension of the lattice and K_1 a Bessel function.

* **Isospin and electromagnetic effects:** Traditionally subdominant, but become important due to reduction of dominant errors.

2.3. Tests of lattice QCD

After determining the **5 parameters of the lattice action** (quark masses ($m_u = m_d$ and a) using 5 experimental quantities as inputs), we can make predictions for all other quantities.

Lattice calculations of all other quantities should agree with experiment.

Simple quantities to calculate using Lattice QCD

For stable (or almost stable) hadrons, masses and amplitudes with no more than one initial (final) state hadron

Including quark masses and α_s , hadron spectrum, weak decays (leptonic, semileptonic, mixing)...

2.3. Tests of lattice QCD

$$V_{CKM} = \left(\begin{array}{ccc}
 |V_{ud}| & |V_{us}| & |V_{ub}| \\
 \pi \rightarrow l\nu & K \rightarrow l\nu & B \rightarrow \tau\nu \\
 & K \rightarrow \pi l\nu & B \rightarrow \pi\tau\nu \\
 |V_{cd}| & |V_{cs}| & |V_{cb}| \\
 D \rightarrow l\nu & D_s \rightarrow l\nu & B \rightarrow Dl\nu \\
 D \rightarrow \pi l\nu & D \rightarrow Kl\nu & B \rightarrow D^*l\nu \\
 |V_{td}| & |V_{ts}| & |V_{tb}| \\
 \langle B_d^0 | \bar{B}_d^0 \rangle & \langle B_s^0 | \bar{B}_s^0 \rangle & \text{no } t\bar{q} \text{ hadrons}
 \end{array} \right) \quad \text{arg}(V_{ub}^*) \quad \langle K^0 | \bar{K}^0 \rangle$$

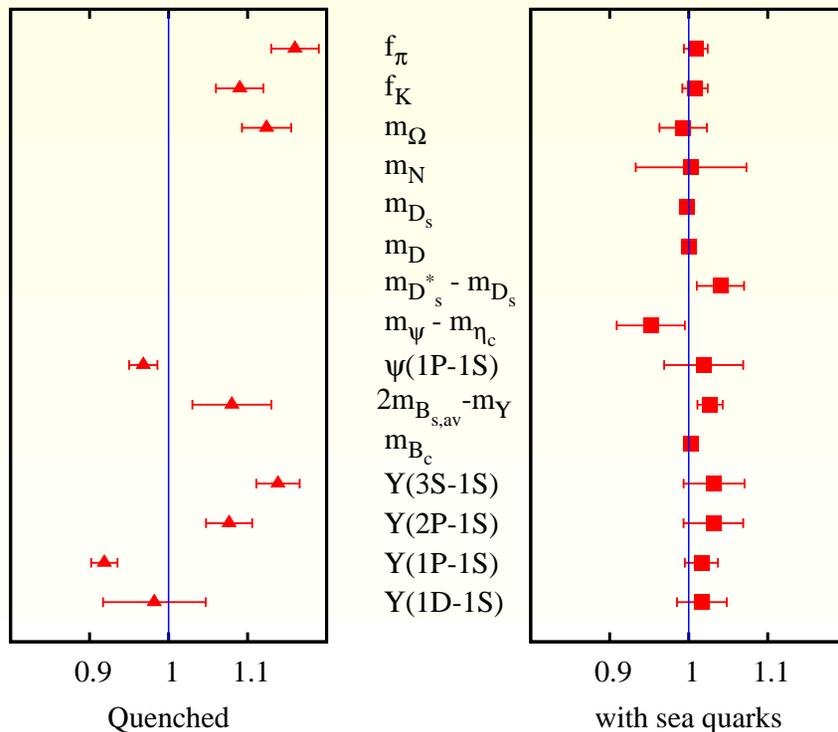
2.3. Tests of lattice QCD

Phenomenology needs precise lattice QCD calculations → Control and reliably estimate systematic errors

In particular, we need **unquenched** calculations.

1999: MILC Started to generate ensembles with $N_f = 2 + 1$ sea quarks, using the Asqtad (staggered) action.

2004: MILC+HPQCD+FNAL Tested them against experiment at the 2-3% level.

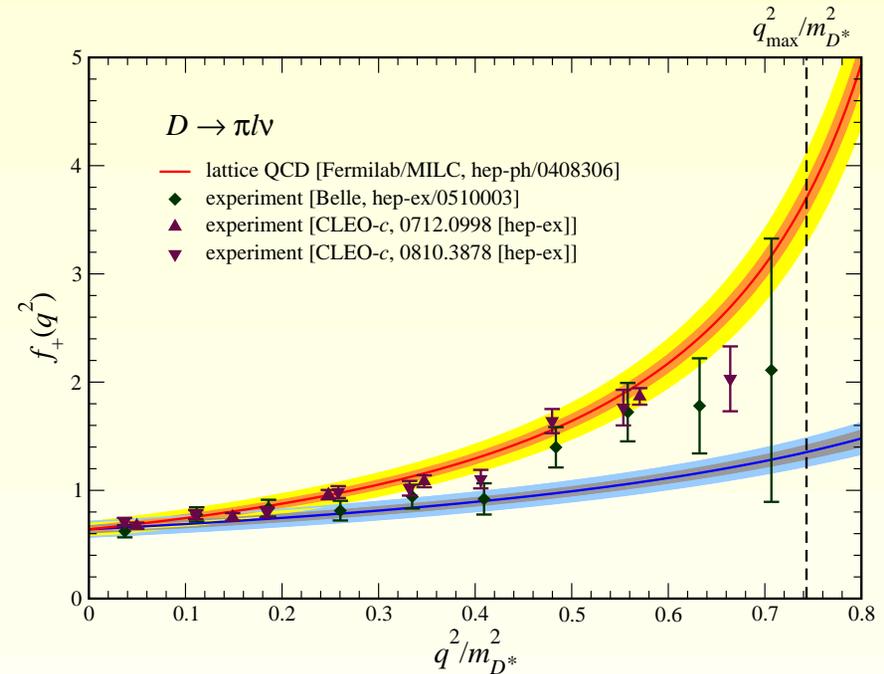
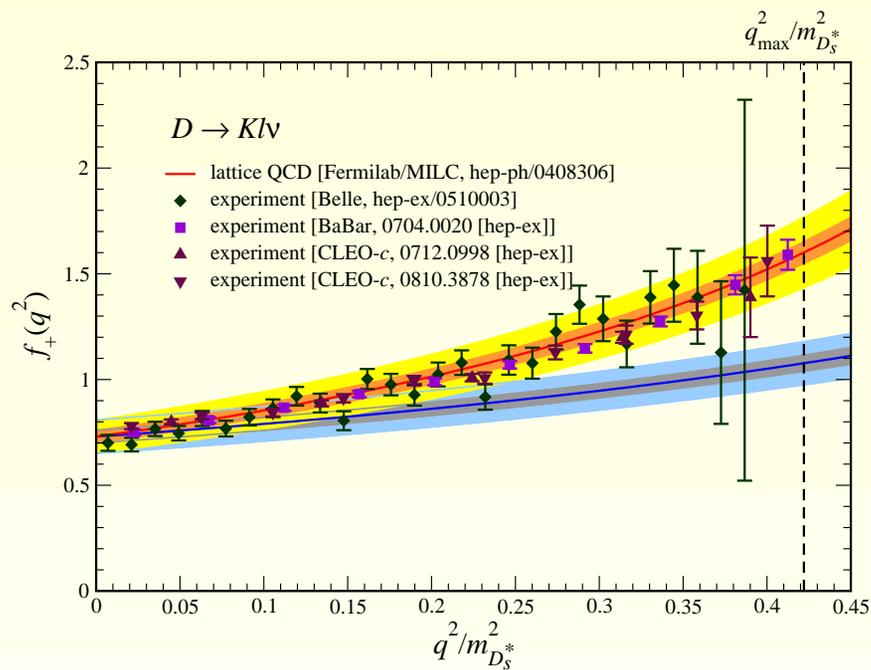


2007 update

2.3. Tests of lattice QCD

2005: FNAL/MILC Predictions for D , D_s meson decays constants and semileptonic form factors (shape) with 7 – 9% precision.

FNAL/MILC and HPQCD, Phys. Rev. Lett. 94:011601,2005



* Normalization agrees with experiment ($|V_{cd(cs)}|$ from elsewhere).

* **Prediction** of the shape.

2005: FNAL+HPQCD Prediction for B_c mass

2.3. Tests of lattice QCD

2006: **RBC/UKQCD** started to generate $N_f = 2 + 1$ ensembles with **domain wall** fermions.

2007: $N_f = 2 + 1$ ensembles started to be generated by several collaborations (**BMW, PACS-CS, JLQCD/TWQCD, HSC**) using different gauge and fermion actions.

2008: **BMW, PACS-CS, MILC** predictions of the light hadron spectrum. Also some results from **HSC, HLPC**.

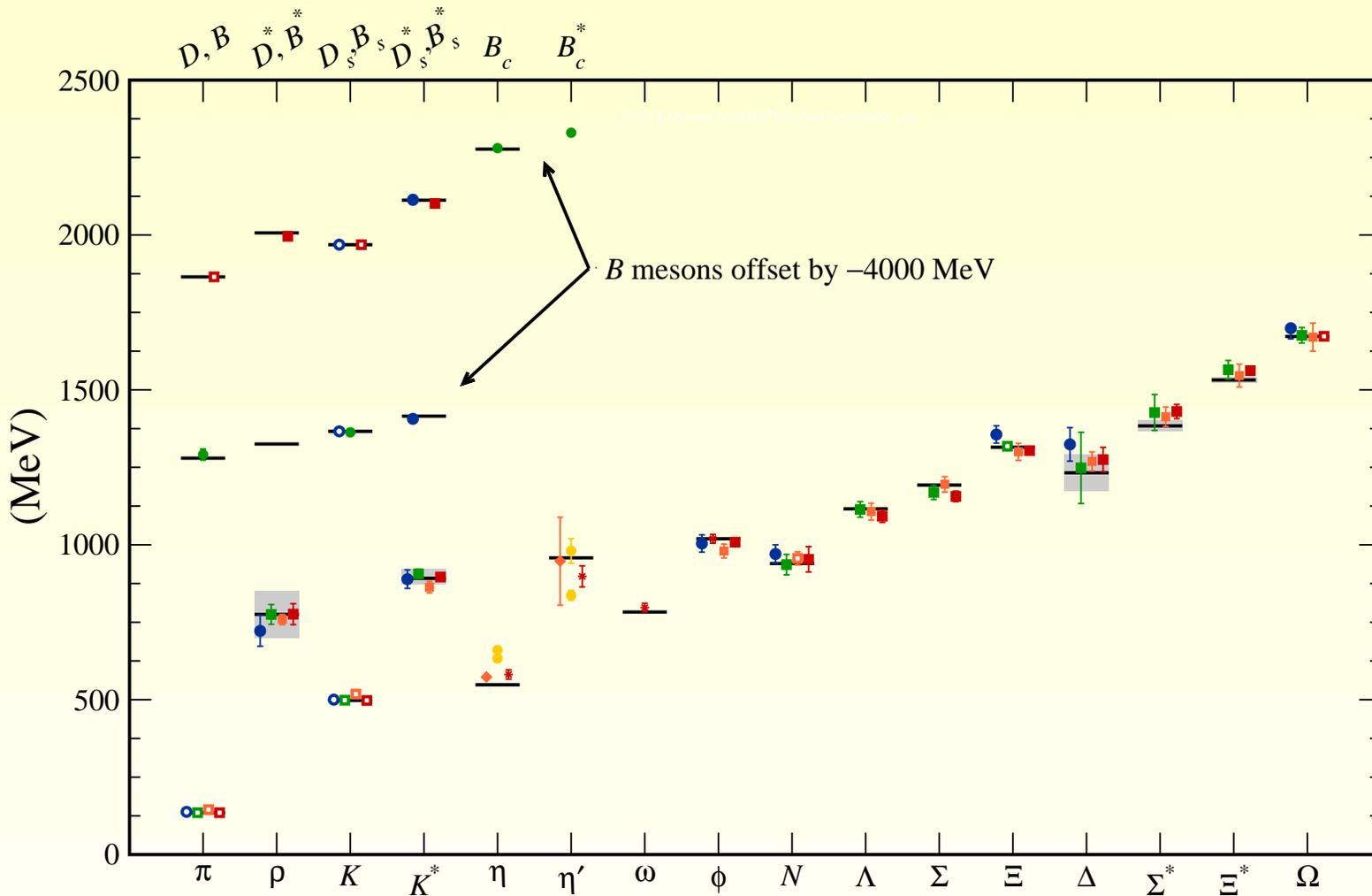
$N_f = 2 + 1 + 1$ ensembles starting to be generated

2010-2011:

BMW, PACS-CS, FNAL/MILC First physical results at the physical light quark masses.

ETMC and **FNAL/MILC** First physical results on $N_f = 2 + 1 + 1$ ensembles.

2.3.1. Tests of lattice QCD: hadron spectrum



$\pi \dots \Omega$: BMW, MILC, PACS-CS, QCDSF

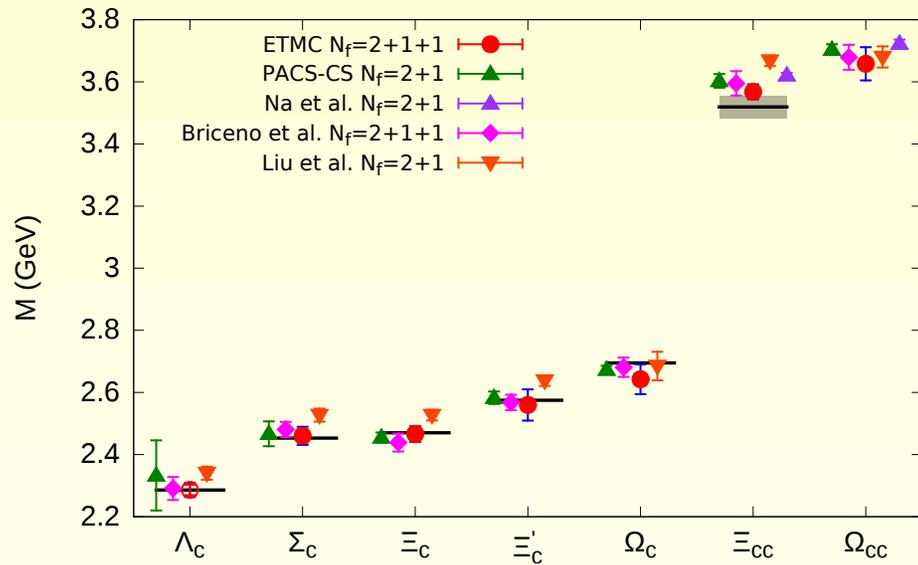
Black lines: experiment

η, η' : RBC UKQCD Hadron spectrum (ω)

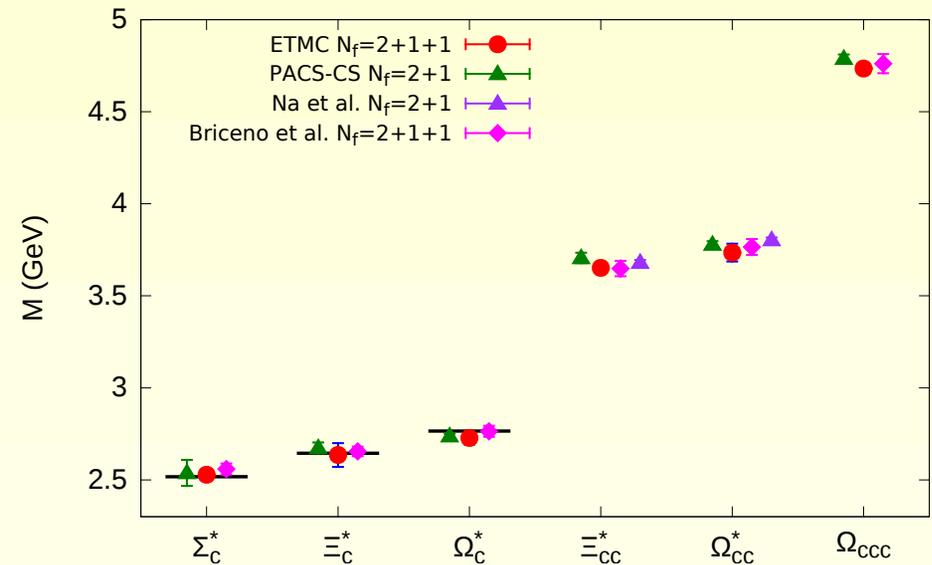
D, B : Fermilab, HPQCD, Mohler-Woloshyn

2.3. Tests of lattice QCD: hadron spectrum

C. Alexandrou et al (ETM), arXiv:1406.4310



$S = 1/2$



$S = 3/2$

2.4. Determination of fundamental parameters: quark masses and α_s

Once the parameters of the lattice lagrangian (lattice spacing (\equiv scale) and bare quark masses) are fixed, we can get the corresponding physical quantities.

Quark masses in a lattice simulation, am_q^{lat} , are bare parameters defined in the lattice regularization scheme and depend on the fermion action and the lattice scale.

→ Go to a continuum scheme: **renormalization**

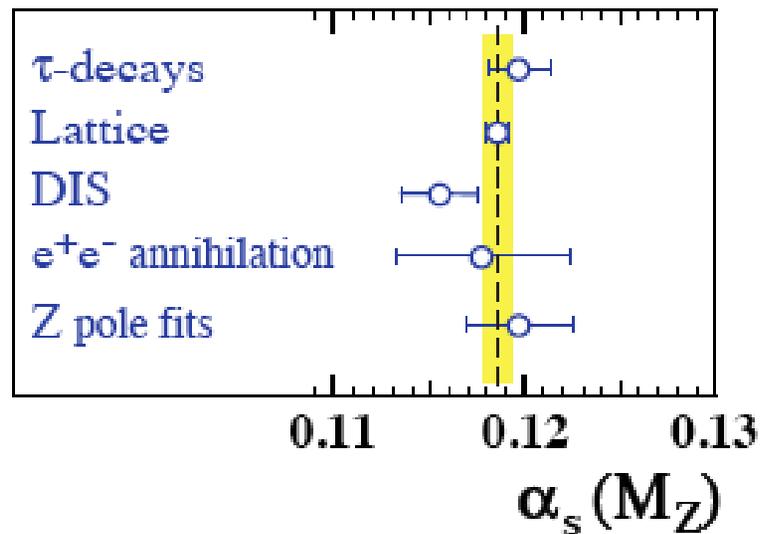
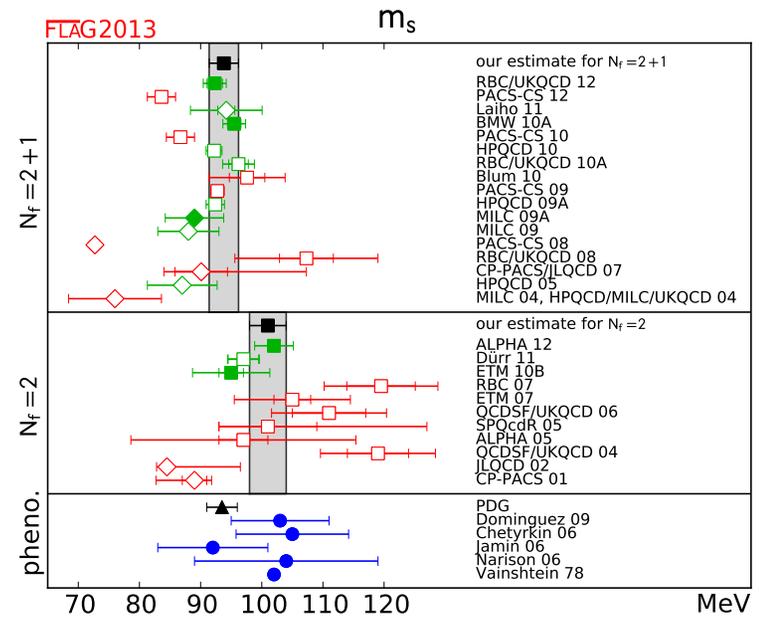
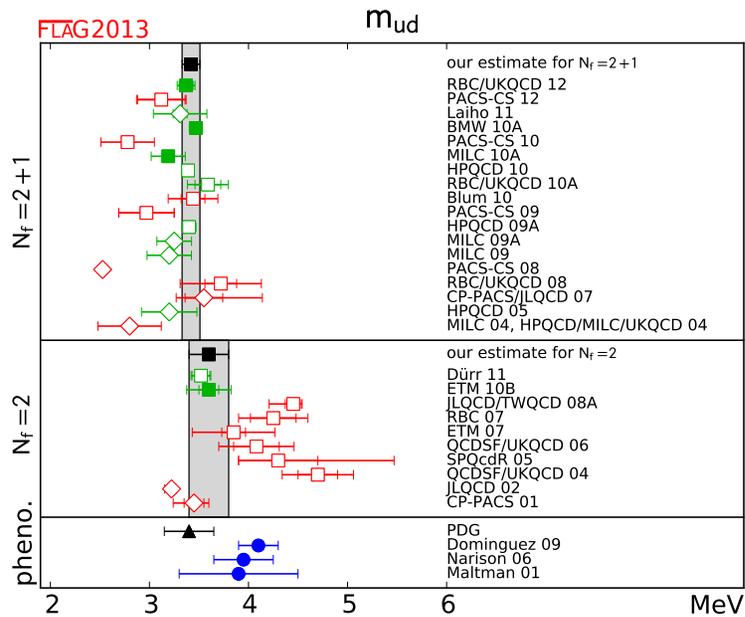
$$m_q^{\overline{MS}}(\mu) = Z^{\overline{MS},\text{lat.}}(\mu a, m_q^{\text{latt}} a) \frac{1}{a} am_q^{\text{lat}}$$

* Perturbatively: Up to two loops $Z = 1 + \alpha_s z_1^{(1)} + \alpha_s^2 z_1^{(2)} + \dots$

** Lattice perturbative calculations highly non-trivial and for m_q needs at least two-loops.

* Non-perturbatively: Z will have statistical and systematic errors.

2.4. Determination of fundamental parameters: quark masses and α_s



PDG2014

2.4. Determination of fundamental parameters: quark masses and α_s

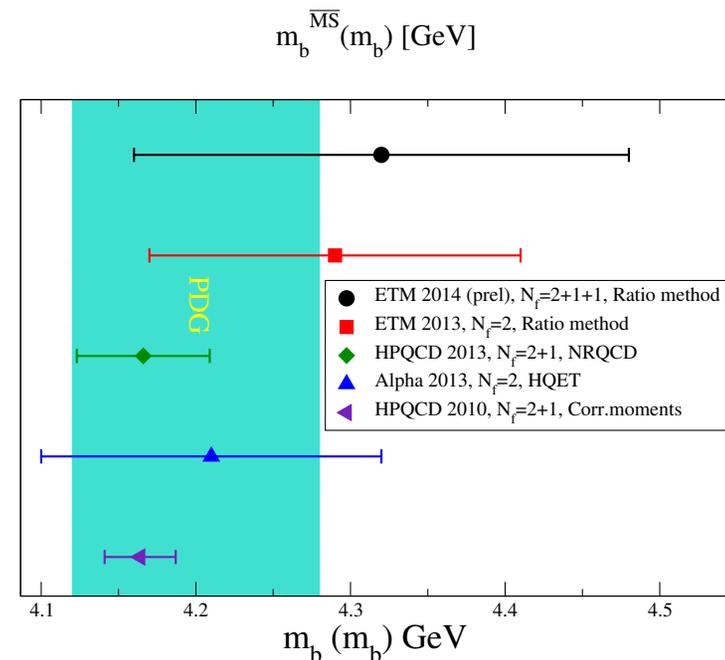
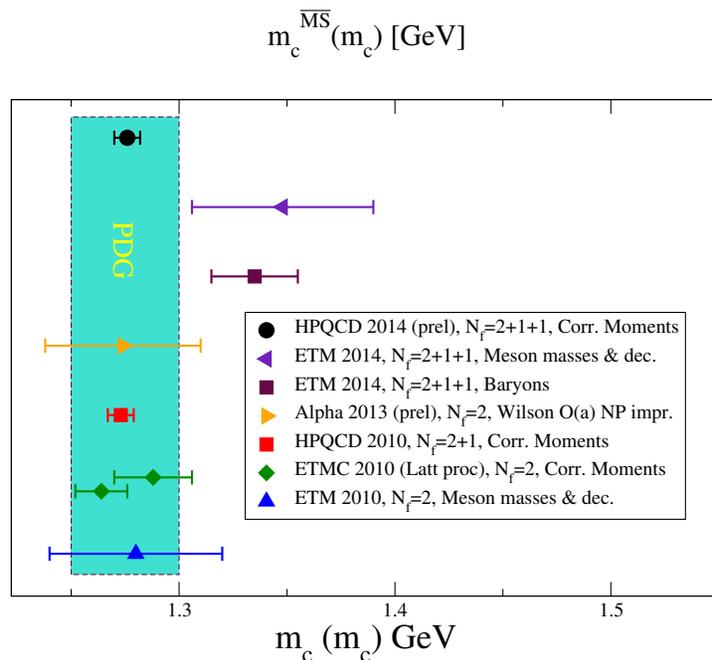
Alternatively for $m_h = m_c, m_b$: Use dispersion relations involving correlation functions calculated on the lattice and perturbative expansions in the continuum.

Example:

$$G_n \equiv \sum_t (t/a)^n G(t) \quad \text{with} \quad G(t) \equiv a^6 \sum_{\vec{x}} (am_{0h})^2 \langle 0 | j_5(\vec{x}, t) j_5(0, 0) | 0 \rangle$$

$$\underbrace{G_n}_{\text{lattice}} = \frac{g_n(\alpha_s^{\overline{MS}}(\mu), \mu/m_h)}{\left(am_h^{\overline{MS}}(\mu)\right)^{n-4}} \rightarrow m_h^{\overline{MS}}(\mu), \alpha_s^{\overline{MS}}(\mu)$$

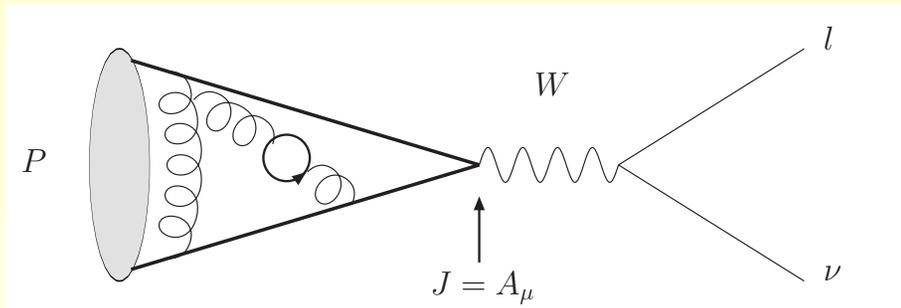
review by **F. Sanfilippo** at Lattice2014



3. Flavour physics on the lattice: examples

3.1. Decay constants

Purely leptonic decays can be used to extract **CKM** matrix **elements** or to test **SM/lattice** predictions



$$\underbrace{\Gamma(P \rightarrow l\nu)}_{\text{experiment}} \propto |V_{ab}|^2 \underbrace{f_P^2}_{\text{lattice}}$$

Simple matrix element $\langle 0 | \bar{a} \gamma_\mu \gamma_5 b | P(p) \rangle = i f_P p_\mu \rightarrow$ precise calculations

$$\left(\text{or } (m_a + m_b) \langle 0 | \bar{a} \gamma_5 b | P(p=0) \rangle = f_P M_P^2 \right)$$

* On the lattice, we calculate 2-point correlation functions

$$C_2(t) = \frac{1}{L^3} \sum_{\vec{y}} \langle 0 | \mathcal{O}(\vec{y}, t) \mathcal{O}(\vec{0}, 0) | 0 \rangle = C_{PP} e^{-M_P t} + \text{excited states}$$

from which we extract C_{PP} and M_P , and get the decay constant as

$$f_P = (m_a + m_b) \sqrt{\frac{L^3}{4}} \sqrt{\frac{C_{PP}}{M_P^3}}$$

3.1. Decay constants

Remember:

$$\sum_{\vec{y}} \langle 0 | \mathcal{O}(\vec{y}, 0) \mathcal{O}(\vec{0}, t) | 0 \rangle = \int \mathcal{D}U \text{Tr}_{\text{spin,color},\tilde{y}} \left[M_{y,0}^{-1,a}(A) \gamma_5 M_{0,y}^{-1,b}(A) \gamma_5 \right] e^{-S_{eff}}$$

(with $M_{x,y}^{-1,a}$ the propagator of a quark of flavour a from x to y)

is evaluated on sets of configurations U 's distributed according to $e^{-S_{eff}}$.

3.1.1. Decay constants of D and D_s mesons

Example calculation from [A. Bazavov et al, arXiv:1407.3772](#) (simplified version)

- * **MILC** $N_f = 2 + 1 + 1$ ensembles: Highly Improved Staggered quarks (HISQ action) and one-loop tadpole improved Symanzik improved gauge action.
 ~ 1000 configurations on each ensemble.
- * **On the sea sector (configurations)**: Four different values of a and three different values of $m_l = m_d = m_u$, including the physical value, for each a . m_s and m_c close to their physical values.
- * **On the valence sector (for each choice of parameters in the sea sector)**:
For a $c\bar{q}$ meson, 10 different values of m_q ranging from m_l to m_s and 2 values of m_c (one equal to the one in the sea).
- * Three different volumes for one of the ensembles (choice of a and quark masses)

For each choice of parameters above, $C_2(t)$ on each configuration

- extract the aM_D and af_D (and statistical error) for each data point by fitting to the expected theoretical form

3.1.1. Decay constants of D and D_s mesons

Need to extrapolate all the lattice data to the continuum ($a = 0$) and infinite volume limits, and interpolate to the physical quark masses.

Use an **effective field theory** incorporating chiral, a^2 , and finite volume effects systematically: **Staggered Heavy Meson ChPT (SHMChPT)**.

* **Allow to use all data** (included unphys. quark masses):

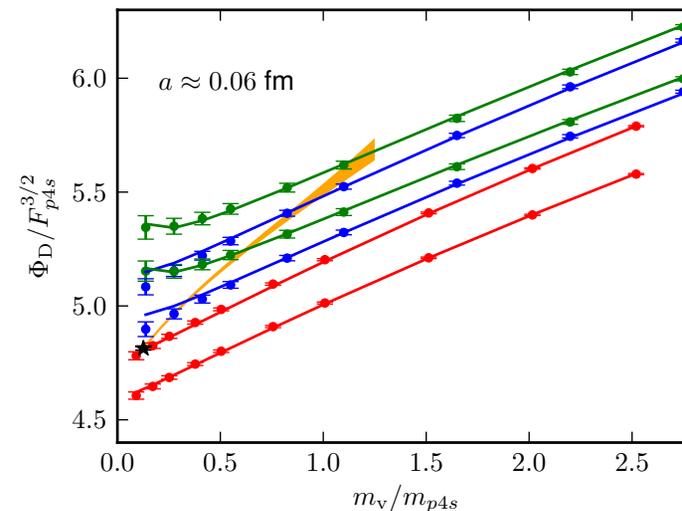
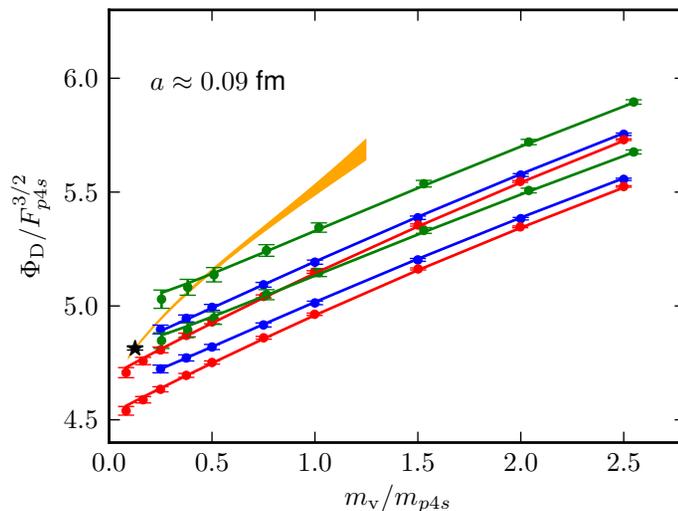
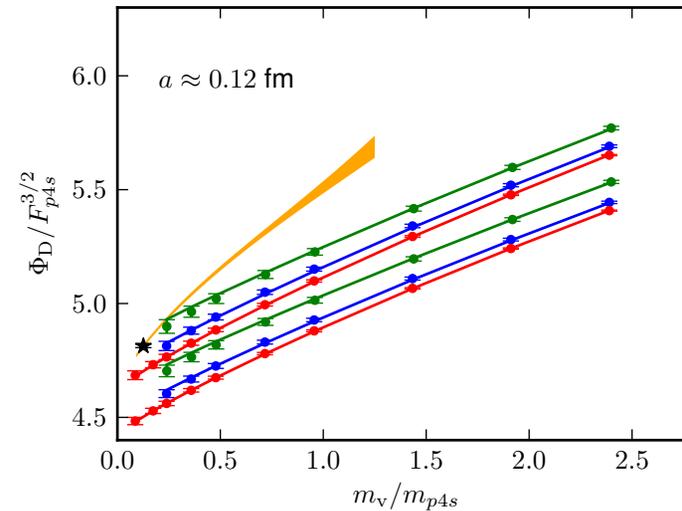
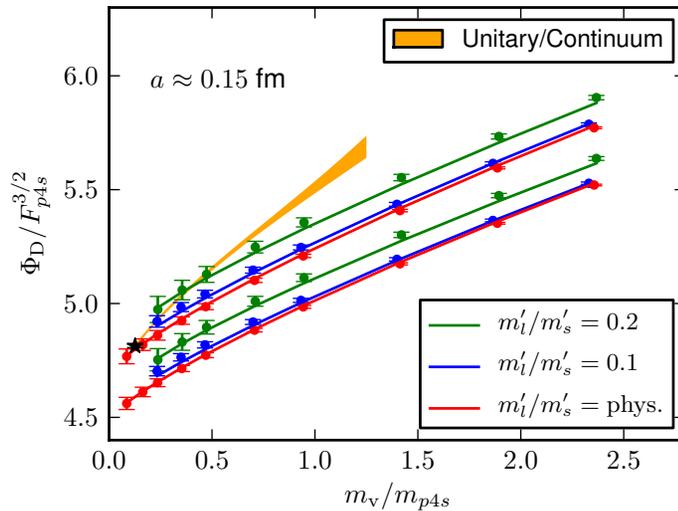
** Reduce statistical errors

** Correct for quark mass mistuning

** Perform continuum and infinite volume extrapolation in a controlled way

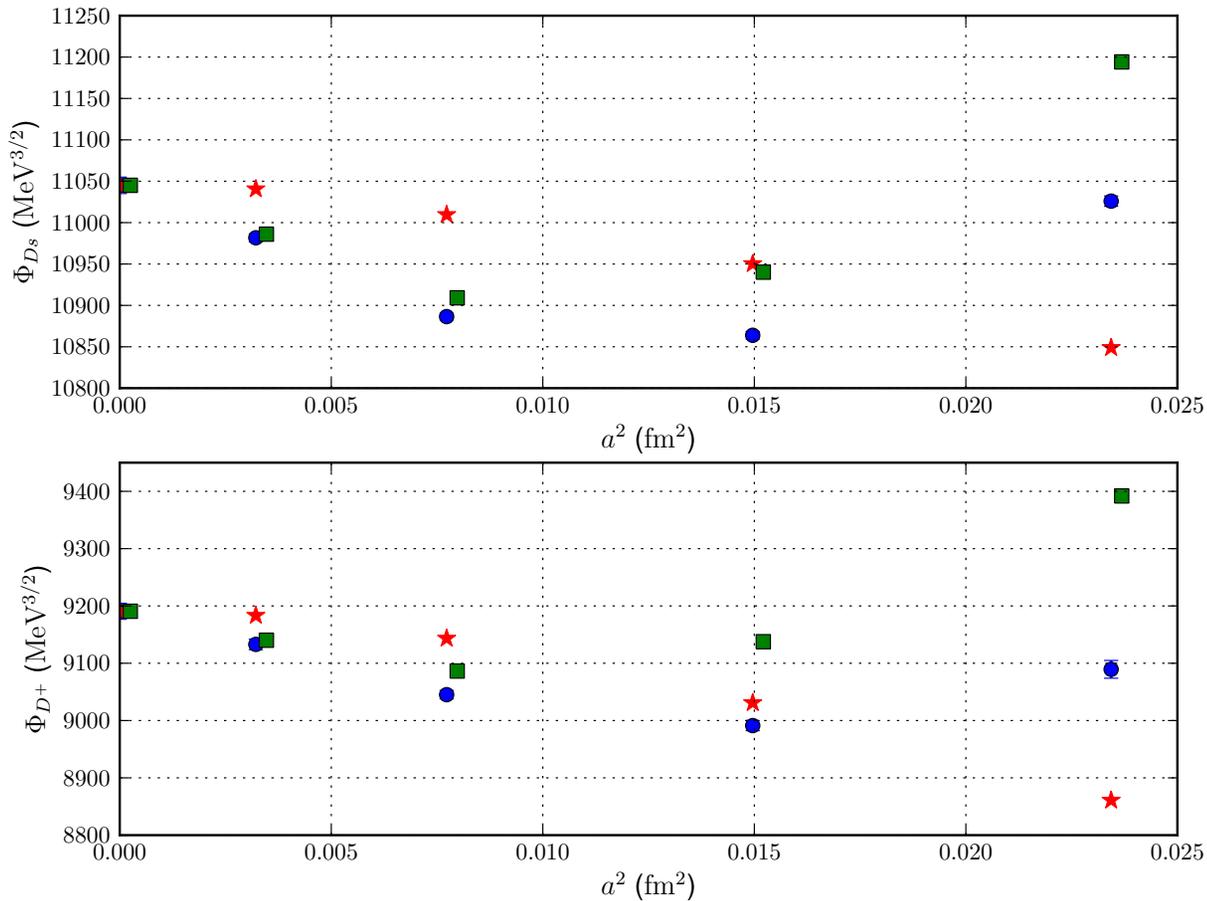
3.1.1. Decay constants of D and D_s mesons

Orange band: Fit result for $\Phi_D = f_D \sqrt{M_D}$ after doing $a = 0$, $m_v = m_l$, and adjusting m_s and m_c to their physical values.



$m_v \equiv$ valence quark mass between $\approx m_l$ and $\approx m_s$. $m'_{l,s}$ are sea quark masses.

3.1.1. Decay constants of D and D_s mesons



- data (interpolated to physical quark masses)
- Contribution from staggered chiral logarithms.
- Contribution from analytical terms $\alpha_s a^2$, $\alpha_s^2 a^2$, a^4 .

3.1.1. Decay constants of D and D_s mesons

Final results:

$$f_{D^+} = 212.6 \pm 0.4_{\text{stat}} \left. \begin{smallmatrix} +0.9 \\ -0.8 \end{smallmatrix} \right|_{a^2} \text{extrap} \pm 0.3_{\text{FV}} \pm 0.0_{\text{EM}} \pm 0.3_{f_\pi \text{ PDG}} \text{ MeV}$$

$$f_{D^+} = 212.6(0.4) \left(\begin{smallmatrix} +1.0 \\ -1.2 \end{smallmatrix} \right) \text{ MeV}$$

$$f_{D_s} = 249.0 \pm 0.3_{\text{stat}} \left. \begin{smallmatrix} +1.0 \\ -0.9 \end{smallmatrix} \right|_{a^2} \text{extrap} \pm 0.2_{\text{FV}} \pm 0.1_{\text{EM}} \pm 0.4_{f_\pi \text{ PDG}} \text{ MeV}$$

$$f_{D_s} = 249.0(0.3) \left(\begin{smallmatrix} +1.1 \\ -1.5 \end{smallmatrix} \right) \text{ MeV}$$

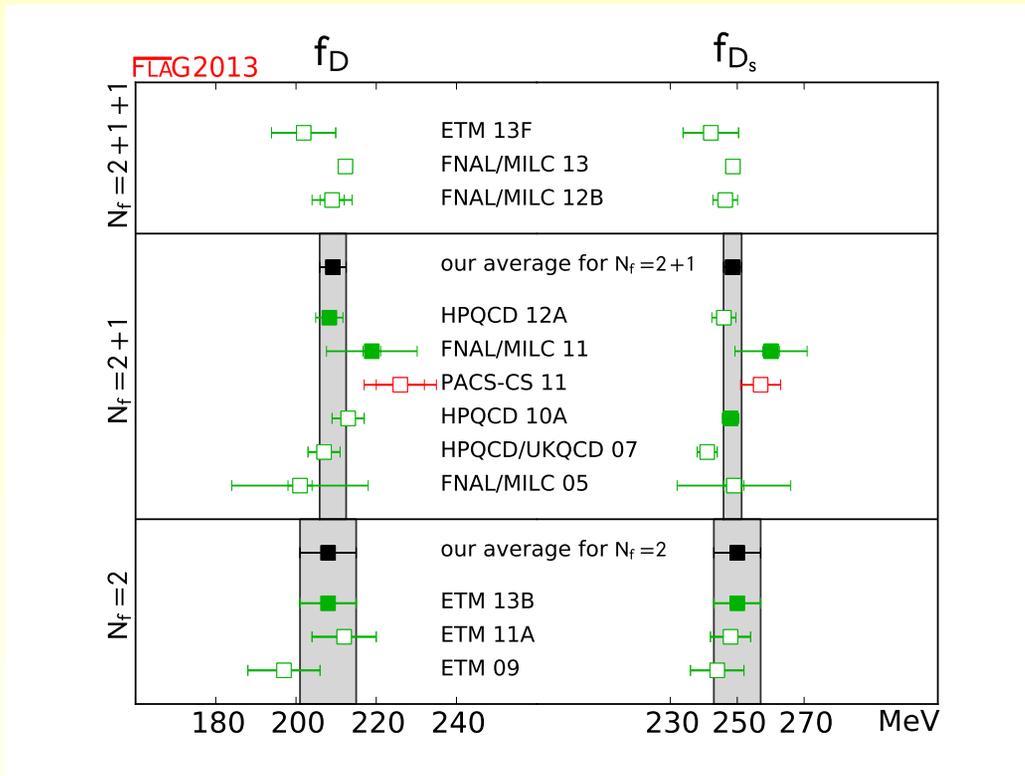
(FV error comes from f_π needed in the scaling setting process, direct FV error is negligible and included in the extrap. error)

Agreement with analysis including only physical quark masses ensembles, but with smaller errors and more robust systematic error analysis.

Need to include the (until recently subdominant) uncertainties from FV and EM effects

3.1.1. Decay constants of D and D_s mesons: summary

Reduction of errors in f_D and f_{D_s} due to the use of relativistic actions.



FLAG – 2, $N_f = 2 + 1$

$$f_D = (209.2 \pm 3.3) \text{ MeV}$$

$$f_{D_s} = (248.6 \pm 2.7) \text{ MeV}$$

experimental averages **Rosner, Stone, Zupanc, CKM 2014**

$$f_D = (203.9 \pm 4.7) \text{ MeV}$$

$$f_{D_s} = (256.9 \pm 4.4) \text{ MeV}$$

(using $|V_{cs}|, |V_{cd}|$ from global SM fit and experimentally measured $\Gamma(D, D_s \rightarrow l\nu)$)

FNAL/MILC 13: Calculation in previous slides.

$$f_{D^+} = 212.6^{(+1.1)}_{(-1.3)} \text{ MeV}$$

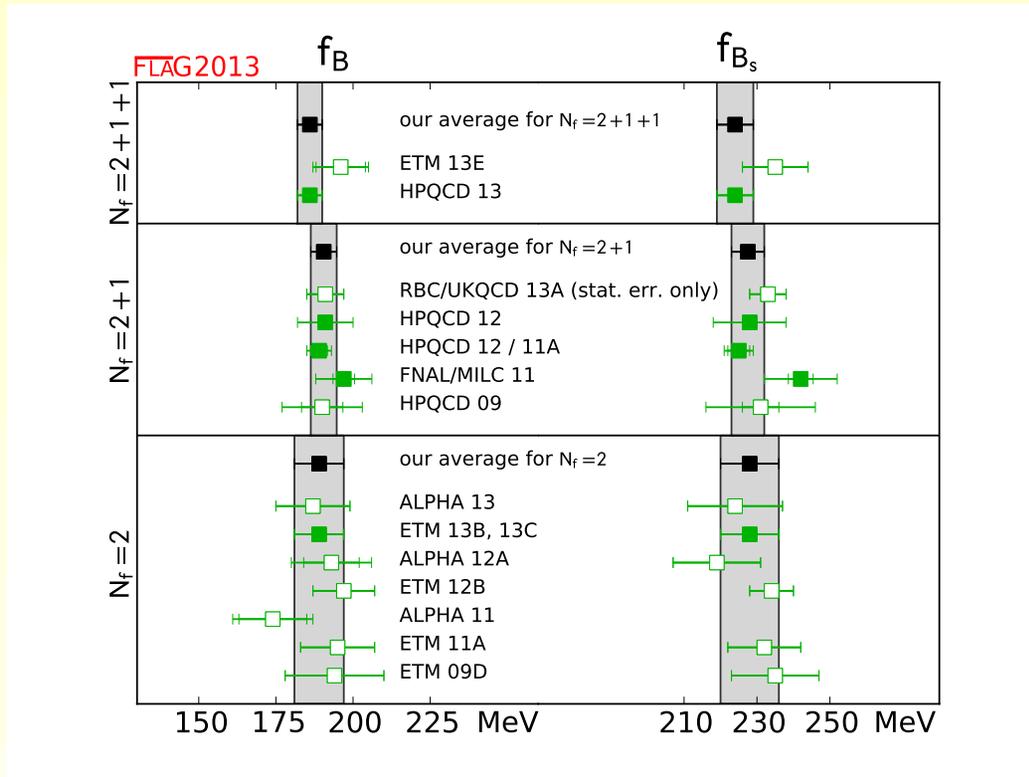
$$f_{D_s} = 249.0^{(+1.1)}_{(-1.5)} \text{ MeV}$$

Small errors due to: highly improved action, physical light quark masses, no renormalization, MILC ensembles with small lattice spacing (0.06 fm)

3.1.2. Decay constants of B and B_s mesons: summary

- # Needed for processes potentially sensitive to NP: $B_{(s)} \rightarrow \mu^+ \mu^-$.
- # Check agreement theory-experiment $Br(B^- \rightarrow \tau^- \bar{\nu}_\tau)$.
- # UT inputs.

3.1.2. Decay constants of B and B_s mesons: summary



FLAG-2

$$f_B^{N_f=2+1+1} = (186 \pm 4) \text{ MeV}$$

$$f_{B_s}^{N_f=2+1+1} = (224 \pm 5) \text{ MeV}$$

$$f_B^{N_f=2+1} = (190.5 \pm 4.2) \text{ MeV}$$

$$f_{B_s}^{N_f=2+1} = (227.7 \pm 4.5) \text{ MeV}$$

$$[f_B^{N_f=2} = (189 \pm 8) \text{ MeV},$$

$$f_{B_s}^{N_f=2} = (228 \pm 8) \text{ MeV}]$$

Using $f_B^{N_f=2+1}$ above: $Br(B^+ \rightarrow \tau\nu)/|V_{ub}|^2 = 6.42(21)$

Belle av.: $Br(B^+ \rightarrow \tau\nu)/|V_{ub}^{exc.}|^2 = 8.2 \pm 3.1;$

$Br(B^+ \rightarrow \tau\nu)/|V_{ub}^{inc.}|^2 = 5.0 \pm 1.7$

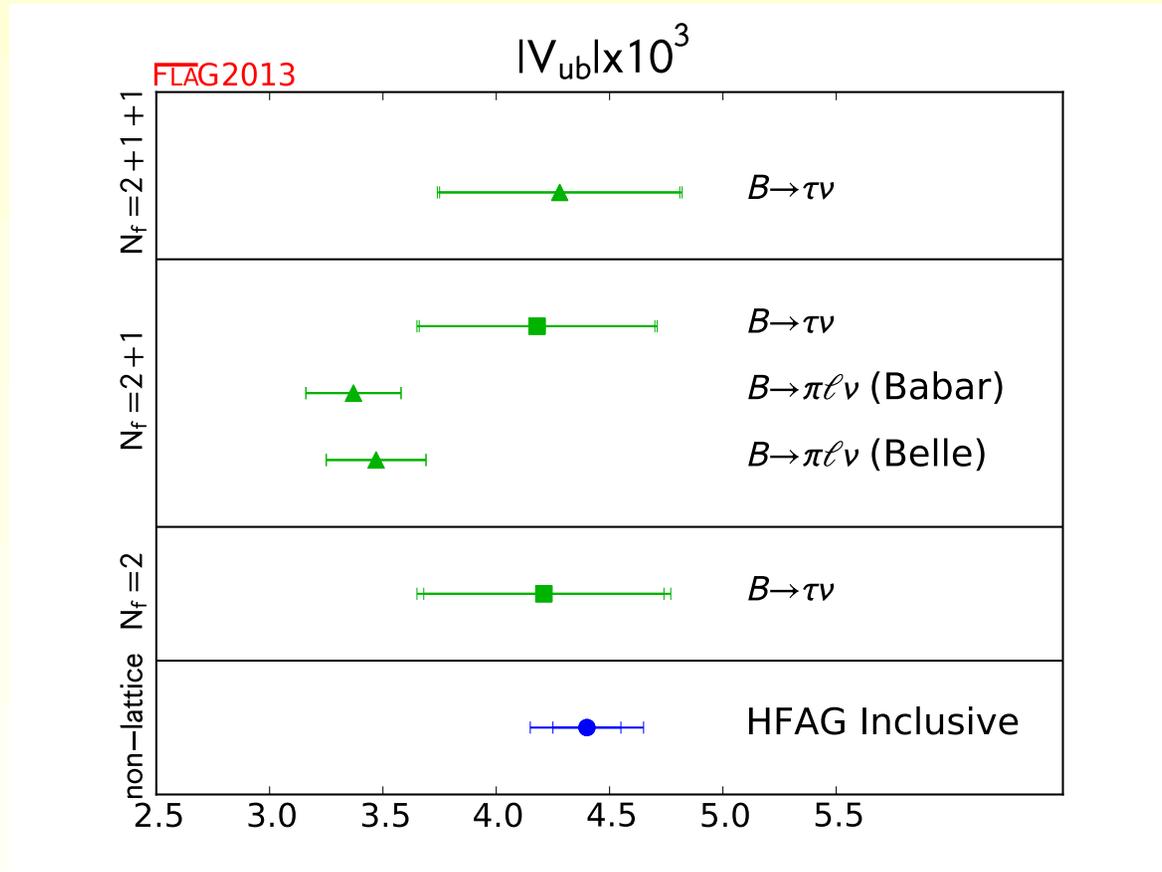
BaBar av.: $Br(B^+ \rightarrow \tau\nu)/|V_{ub}^{exc.}|^2 = 15.3 \pm 4.2;$

$Br(B^+ \rightarrow \tau\nu)/|V_{ub}^{inc.}|^2 = 9.2 \pm 2.3$

exp. averages from Rosner and Stone, 1309.1924

3.1.2. Decay constants of B and B_s mesons

Conversely, extract the value of $|V_{ub}|$ from $f_B^{lattice}$ and experimental measurements of $B \rightarrow \tau\nu$:



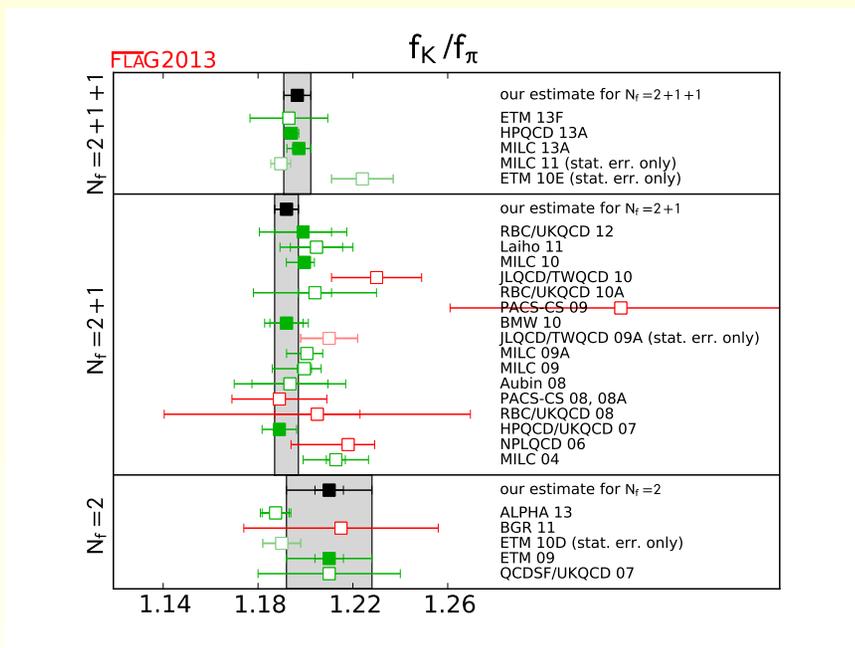
3σ tension between exclusive and inclusive determinations

Exc. determination: Use experimental data on $B \rightarrow \pi l \nu$ and non-perturbative inputs (form factors) from lattice QCD.

3.1.3. Ratios of decay constants: f_K/f_π and $|V_{us}|$

For ratios of decay constants, higher precision can be achieved due to cancellation of statistics and systematics uncertainties.

Many $N_f = 2 + 1, 2 + 1 + 1$ calculations of $f_K/f_\pi \rightarrow$ good test of LQCD



$$f_{K^\pm} / f_{\pi^\pm}^{N_f=2+1+1} = 1.194(5)$$

$$f_{K^\pm} / f_{\pi^\pm}^{N_f=2+1} = 1.192(5)$$

Marciano (2005) proposed to extract the CKM element $|V_{us}|$ from

$$\underbrace{\frac{\Gamma(K \rightarrow \mu \bar{\nu}_\mu(\gamma))}{\Gamma(\pi \rightarrow \mu \bar{\nu}_\mu(\gamma))}}_{\text{experiment}} \propto \frac{|V_{us}|^2}{|V_{ud}|^2} \underbrace{\left(\frac{f_K}{f_\pi}\right)^2}_{\text{lattice}}$$

3.1.3. Ratios of decay constants: f_K/f_π and $|V_{us}|$

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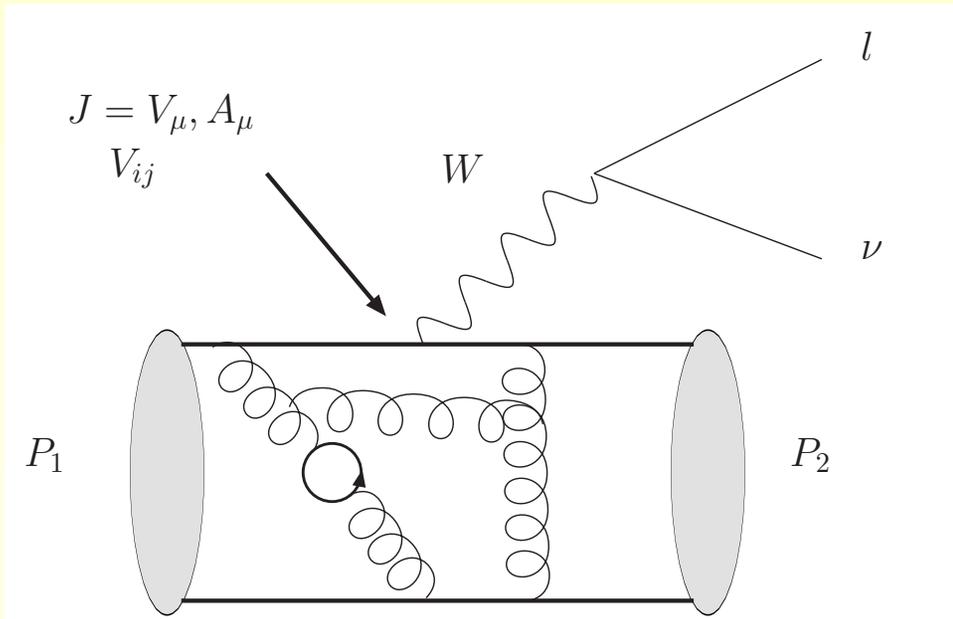
$$\underbrace{\frac{\Gamma(K \rightarrow \mu \bar{\nu}_\mu (\gamma))}{\Gamma(\pi \rightarrow \mu \bar{\nu}_\mu (\gamma))}}_{\text{experiment}} \propto \frac{|V_{us}|^2}{|V_{ud}|^2} \underbrace{\left(\frac{f_K}{f_\pi}\right)^2}_{\text{lattice}}$$

Using the most recent $N_f = 2 + 1 + 1$ lattice calculation **FNAL/MILC2013**, $f_{K^+}/f_{\pi^+} = 1.1956^{(+28)}_{(-34)}$, and experimental data, and $|V_{ud}|$ from nuclear β decays

$$\rightarrow |V_{us}| = 0.22487(51)_{LQCD}(29)_{Br(K_{l2})}(20)_{EM}(5)_{V_{ud}}$$

Further improvements underway, but will eventually require **inclusion of QED** in simulations.

3.2. Semileptonic decays: Extraction of CKM elements



$$\underbrace{\Gamma(P_1 \rightarrow P_2 l \nu)}_{\text{experimental}} \propto |V_{ab}|^2 \underbrace{|f_+(q^2)|^2}_{\text{lattice}}$$

$$\langle P_2(p') | V_\mu | P_1(p) \rangle = (p_\mu + p'_\mu) f_+(q^2) + (p_\mu - p'_\mu) f_-(q^2)$$

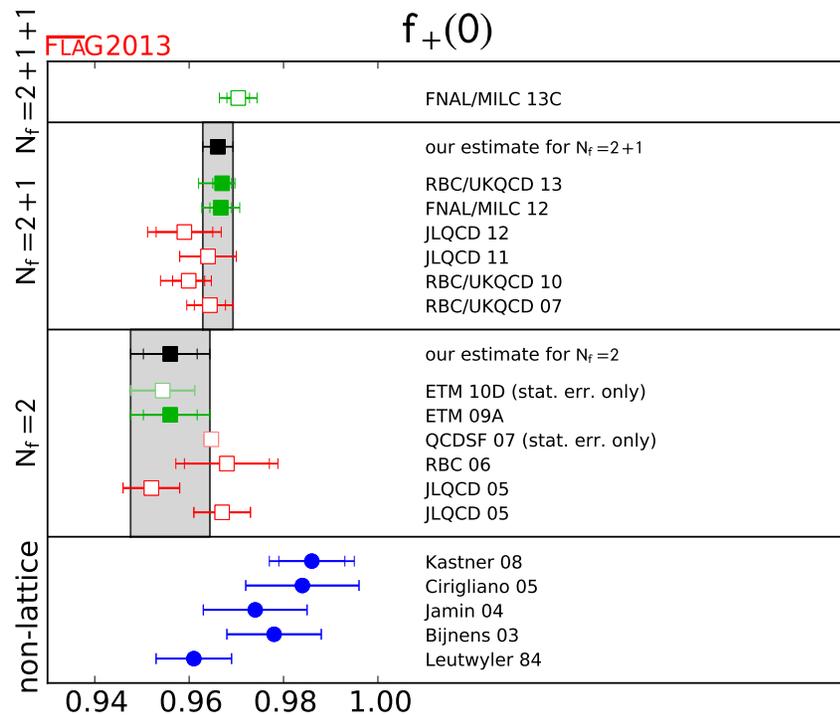
where $q = p - p'$.

- * Extract CKM matrix elements.
- * Testing lattice QCD: shape of the form factor (as a q^2 function) against exper.
- * Correlated signals of NP to those in leptonic decays.

More challenging (and expensive) lattice calculations: 3-point correlation functions, non-zero momentum (discretization errors proportional to $a\vec{p}$), small overlap with experiment in q^2 ...

3.2.1 Semileptonic decays: $K \rightarrow \pi l \nu$ and $|V_{us}|$

Need the form factor at $q^2 = 0$, $f_+^{K\pi}(q^2 = 0)$: very accurate calculation due to vector current conservation in the isospin limit (we calculate isospin corrections of order 2 to $f_+(0) = 1$)



Most precise value is from

FNAL/MILC,

$$f_+(0)^{N_f=2+1+1} = 0.9704(32)$$

with a 0.33% total error

Together with most recent experiment. results for $\Gamma(K \rightarrow \pi l \nu)$

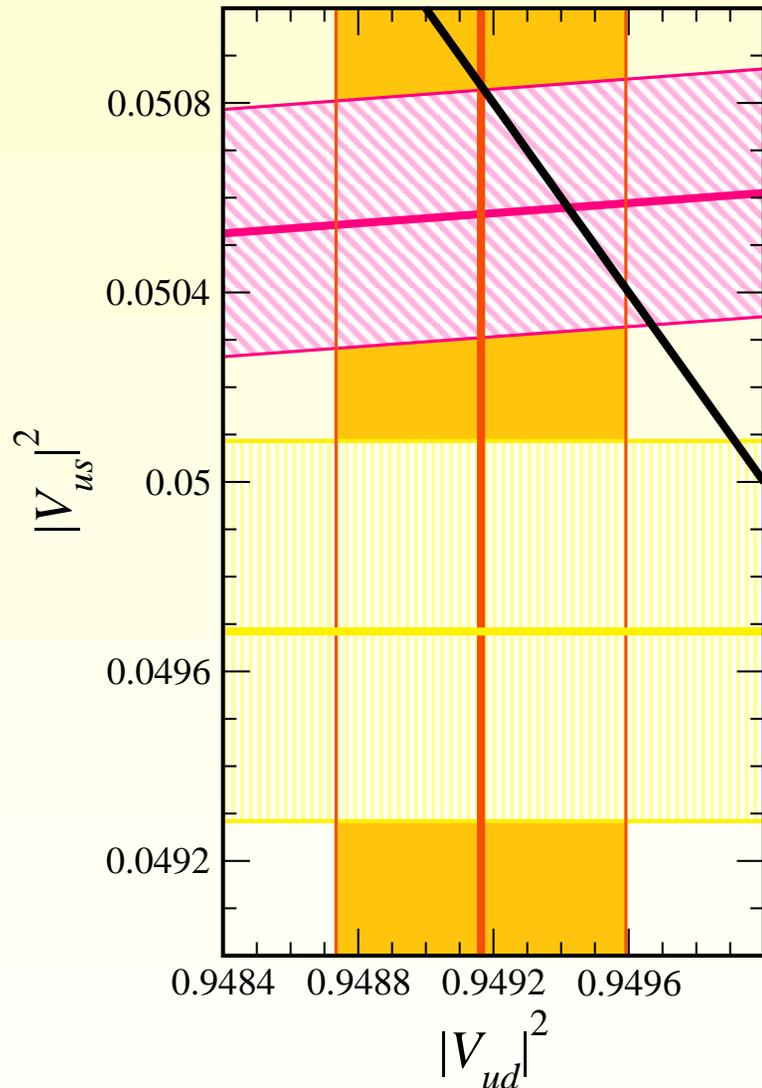
$$|V_{us}| = 0.22290(74) f_+(0) (52)_{expt}$$

How does this value compare with $|V_{us}|$ from leptonic decays?

Does it agree with unitarity?

3.3. Unitarity of the CKM matrix (first row)

Check the unitarity relation $|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 1$.



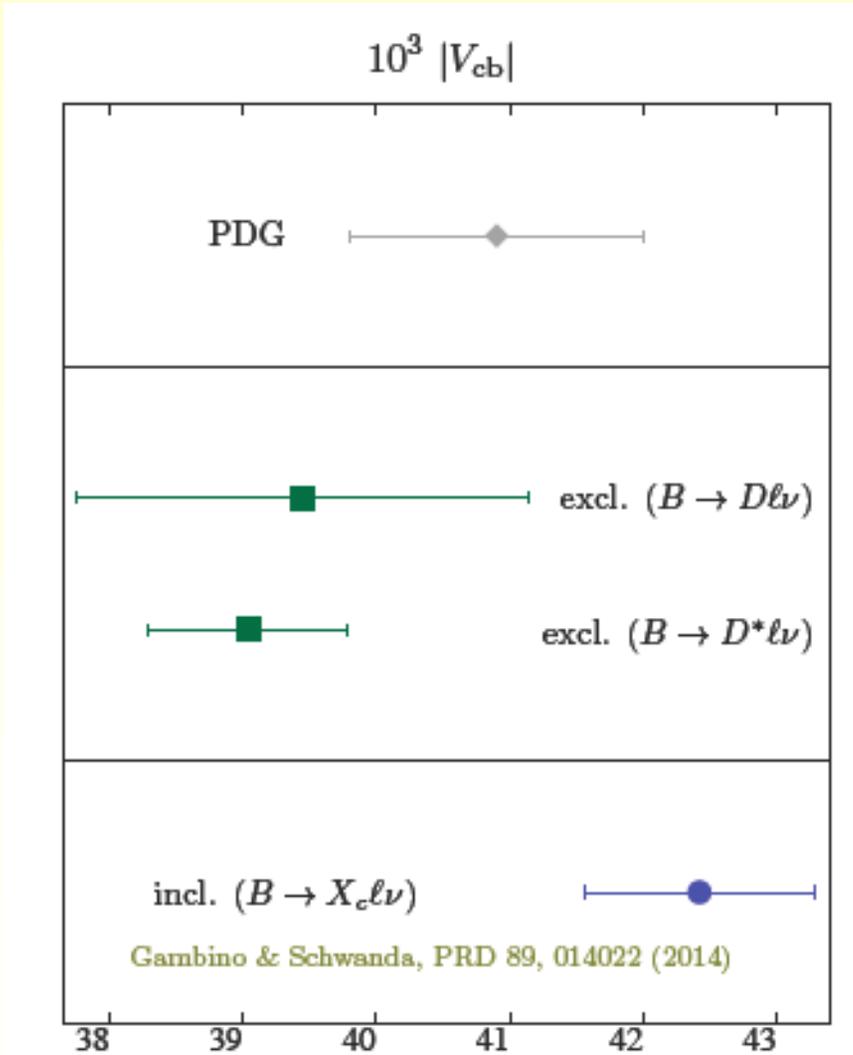
- $|V_{us}|$ (pink) from **FNAL/MILC**
 $N_f = 2 + 1 + 1$ calculation of f_K/f_π and K_{l2} .
- $|V_{us}|$ (orange) from **FNAL/MILC**
 $N_f = 2 + 1 + 1$ calculation of $f_+(0)$ and K_{l3} .
- $|V_{ud}|$ from nuclear beta decays.
- Black line: unitarity line with
 $|V_{ub}| \approx 4 \cdot 10^{-3} \approx 0$

Slight tension between leptonic and semilep.
 V_{us} and between semilep. and unitarity

Uncertainty on $|V_{us}|^2$ at the same order as uncertainty on $|V_{ud}|^2$
→ time to improve $|V_{ud}|$ determinations

3.4. Exclusive vs inclusive determinations of $|V_{cb}|$

$|V_{cb}|$: The indirect **CP** violation parameter ε_K and rare decays such as $\mathcal{B}(K^+ \rightarrow \pi^+ \nu \bar{\nu})$ or $\mathcal{B}(K_L^0 \rightarrow \nu \bar{\nu})$ depend on $|V_{cb}|^4$.



$|V_{cb}|$ extracted from exclusive B decays
($w = v \cdot v'$ is the velocity transfer)

$$\frac{d\Gamma(B \rightarrow D^* l \nu)}{dw} = (\text{known}) \cdot |V_{cb}|^2 \cdot (w^2 - 1)^{1/2} |\mathcal{F}(w)|^2$$

$$\frac{d\Gamma(B \rightarrow D l \nu)}{dw} = (\text{known}) \cdot |V_{cb}|^2 \cdot (w^2 - 1)^{3/2} |\mathcal{G}(w)|^2$$

$\mathcal{F}(w)$ and $\mathcal{G}(w)$ calculated on the lattice.

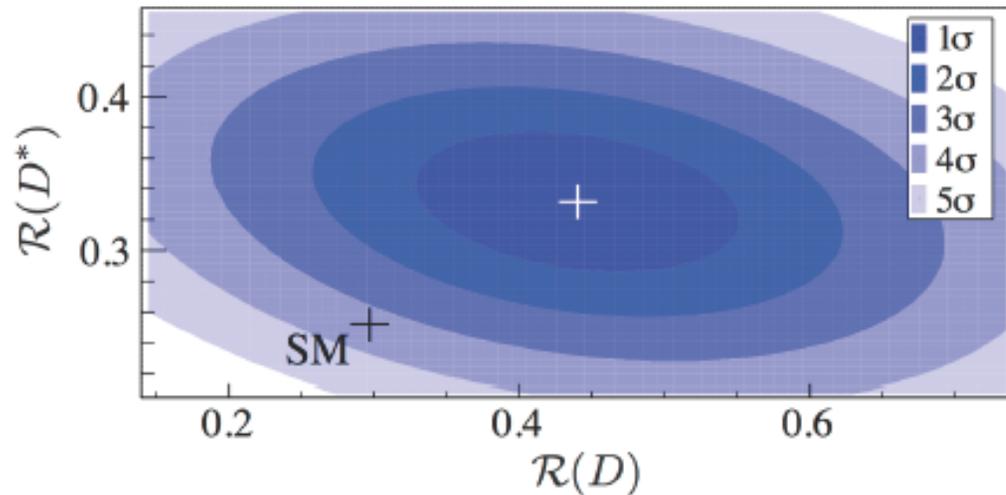
3σ disagreement exc. vs inc.

3.5. BSM phenomenology

(from review by **C. Bouchard** at Lattice 2014)

$$\mathcal{R}(D^{(*)}) = \frac{\mathcal{B}(B \rightarrow D^{(*)}\tau\nu)}{\mathcal{B}(B \rightarrow D^{(*)}\mu\nu)}$$

BaBar, PRD 88, 072012 (2013)



$\mathcal{R}(D)_{\text{SM}}$ from lattice FNAL/MILC, PRL 109, 071802 (2012)

$\mathcal{R}(D^*)_{\text{SM}}$ needs lattice Fajfer et al., PRD 85, 094025 (2012)

$\mathcal{R}(D^*)$ theoretical calculation uses quenched lattice form factors.

$\mathcal{R}(D)$ unquenched prediction is 2σ away from BaBar result

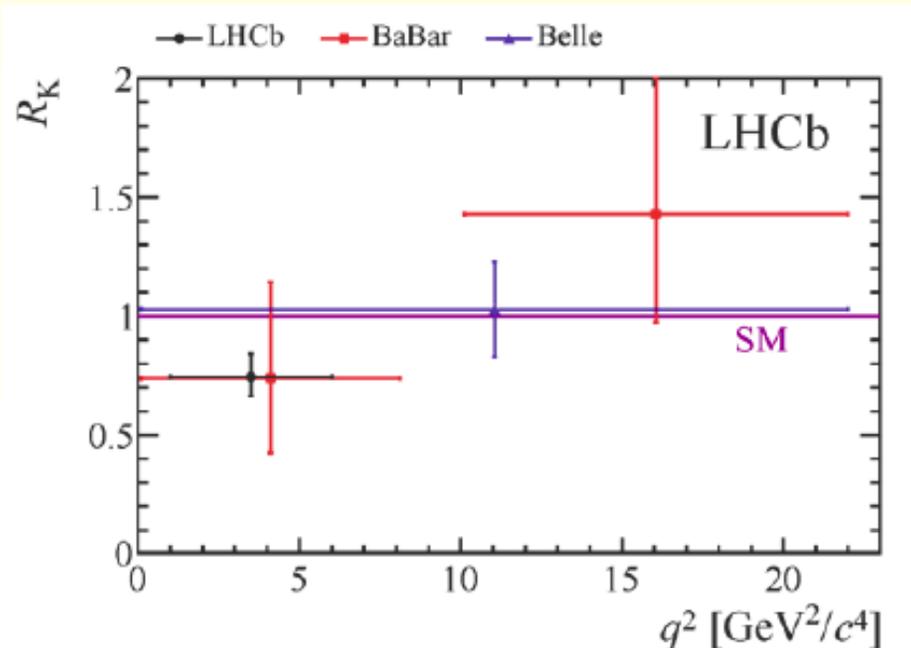
3.5. BSM phenomenology: B rare decays: $B \rightarrow Kll$

First **unquenched** determination of the form factors needed for theoretical prediction: **HPQCD**, arXiv:1306.0434, 1306.2364 (similar to $B \rightarrow \pi l\nu$ but extra tensor form factor)

- * Ratio of branching fractions $B^+ \rightarrow K^+ \mu^+ \mu^-$ and $B^+ \rightarrow K^+ e^+ e^-$, R_K , predicted to be

$$R_K^{lat} = 1.00081(38) \quad (\text{in the range } 1 < q^2 < 6\text{GeV}^2)$$

- * But **LHCb** most recent measurement is $R_K^{exp} = 0.745_{-0.074}^{+0.090} \pm 0.036$



2.6 σ disagreement between LHCb and SM prediction

3.5. BSM phenomenology: B rare decays: $B_{s(d)} \rightarrow \mu^+ \mu^-$

Bag parameters describing B -meson mixing in the SM can be used for theoretical prediction of $\mathcal{B}r(B \rightarrow \mu^+ \mu^-)$ **Buras**, hep-ph/0303060

$$\frac{\mathcal{B}r(B_q \rightarrow \mu^+ \mu^-)}{\Delta M_q} = \tau(B_q) 6\pi \frac{\eta_Y}{\eta_B} \left(\frac{\alpha}{4\pi M_W \sin^2 \theta_W} \right)^2 m_\mu^2 \frac{Y^2(x_t)}{S(x_t)} \frac{1}{\hat{B}_q}$$

* Need to include the effects of a non-vanishing $\Delta\Gamma_s$ to compare with experiment **K. de Bruyn et al.**, 1204.1737

$$\mathcal{B}r(B_q \rightarrow \mu^+ \mu^-)_{SM} \rightarrow \mathcal{B}r(B_q \rightarrow \mu^+ \mu^-)_{y_s} \equiv \mathcal{B}r(B_q \rightarrow \mu^+ \mu^-)_{SM} \times \frac{1}{1-y_s}$$

with $y_s \equiv \Delta\Gamma_s/(2\Gamma_s)$.

* Using $\hat{B}_{B_s} = 1.33(6)$, $\hat{B}_{B_d} = 1.26(11)$ **HPQCD**, 0902.1815, $y_s = 0.087 \pm 0.014$
LHCb, 1212.4140

$$\mathcal{B}r(B_s \rightarrow \mu^+ \mu^-)_{y_s} = (3.71 \pm 0.17) \times 10^{-9} \quad \text{Buras et al. 1303.3820}$$

$$\mathcal{B}r(B_d \rightarrow \mu^+ \mu^-) = (1.03 \pm 0.09) \times 10^{-10}$$

Error dominated by uncertainty in the bag parameter **Buras et al.** 1303.3820

3.5. BSM phenomenology: B rare decays: $B_{s(d)} \rightarrow \mu^+ \mu^-$

Indirect determination

$$\mathcal{B}r(B_s \rightarrow \mu^+ \mu^-)_{y_s} = (3.71 \pm 0.17) \times 10^{-9} \quad \text{Buras et al. 1303.3820}$$

$$\mathcal{B}r(B_d \rightarrow \mu^+ \mu^-) = (1.03 \pm 0.09) \times 10^{-10} \quad \text{Buras et al. 1208.0934}$$

Direct determination using the $N_f = 2 + 1$ lattice averages by FLAG-2 with $N_f = 2 + 1$: $f_B = (190.5 \pm 4.2) \text{ MeV}$ and $f_{B_s} = (227.7 \pm 4.5) \text{ MeV}$.

$$\mathcal{B}r(B_s \rightarrow \mu^+ \mu^-)_{y_s} = (3.65 \pm 0.20) \times 10^{-9} \quad \text{Buras et al. 1303.3820}$$

Dominant errors: $|V_{tb}^* V_{ts}|$ 4%, f_{B_s} 4%

$$\mathcal{B}r(B_d \rightarrow \mu^+ \mu^-) = (1.07 \pm 0.05 \pm 0.05_{f_{B_d}}) \times 10^{-10}$$

Experimental averages LHCb and CMS at CKM2014:

$$\mathcal{B}r(B_s \rightarrow \mu^+ \mu^-) = \left(2.8_{-0.6}^{+0.7}\right) \cdot 10^{-9} \quad \mathcal{B}r(B_d \rightarrow \mu^+ \mu^-) = \left(3.9_{-1.4}^{+1.6}\right) \cdot 10^{-10}$$

There is not space for large effects in B_s^0 system.

In the B_d^0 system, compatibility with SM: 2.2σ

3.6 Beyond simple quantities

When there are two or more hadrons in the final or initial state we need additional formalism to relate quantities calculated in the Euclidean box to physical observables in Minkowski space.

- * $K \rightarrow \pi\pi$

- * Hadronic contributions to muon $g - 2$: hadronic vacuum polarization and hadronic light-by-light contributions can be calculated using lattice methods.

- * Hadron structure and hadronic interactions (for example, π scattering length).

- * Resonances (ρ , K^* and excited charmed mesons widths ...).

Not only QCD: QED, BSM theories (near conformal strong dynamics, composite PNGB-like Higgs, SUSY, Quantum Gravity ...)

4. Conclusions

- * For a more extensive review, see, for example talk by **A. El-Khadra** at ICHEP2014.
- * For a review and averages of the most important lattice results concerning low energy physics see **FLAG-2** website and last review: **S. Aoki et al** arXiv: 1310.8555.
- * For further discussion on specific topics, see talks at **Latttice 2014**: <http://www.bnl.gov/lattice2014/>