Lattice QCD with physical quark masses

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(PLB 705:477,2011, JHEP 1108:148,2011; PLB 701:265,2011;

PRD 81:054507,2010; Science 322:1224,2008)

Purpose of lattice QCD

- QCD fundamental objects: quarks and gluons
- QCD observed objects: protons, neutrons (π, K, ...)

! Huge discrepancy: not even the same particles observed as in the Lagrangean

➛ Perturbation theory has no chance

- Need to solve low energy QCD to:
  - Compute hadronic and nuclear properties
    "people who love QCD"
    - Masses, decay widths, scattering lengths, thermodynamic properties, ...
  - Compute hadronic background
    "people who hate QCD"
    - Non-leptonic weak MEs, quark masses, g-2, ...

Strategy outline

Goal:

- Make ab initio QCD predictions

Step 1: validate (lattice) QCD

- Compute light hadron spectrum

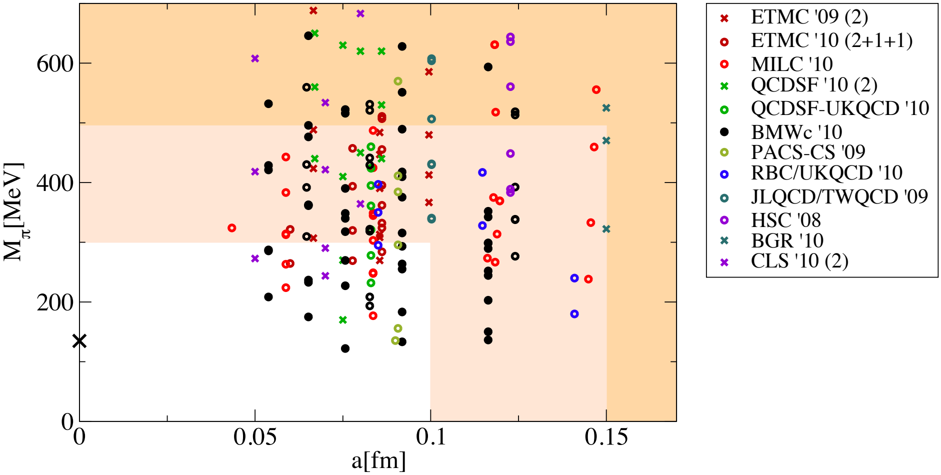
Step 2: Make QCD predictions

- Pseudoscalar decay constant ratio (CKM)
- Light quark masses
- Neutral kaon mixing

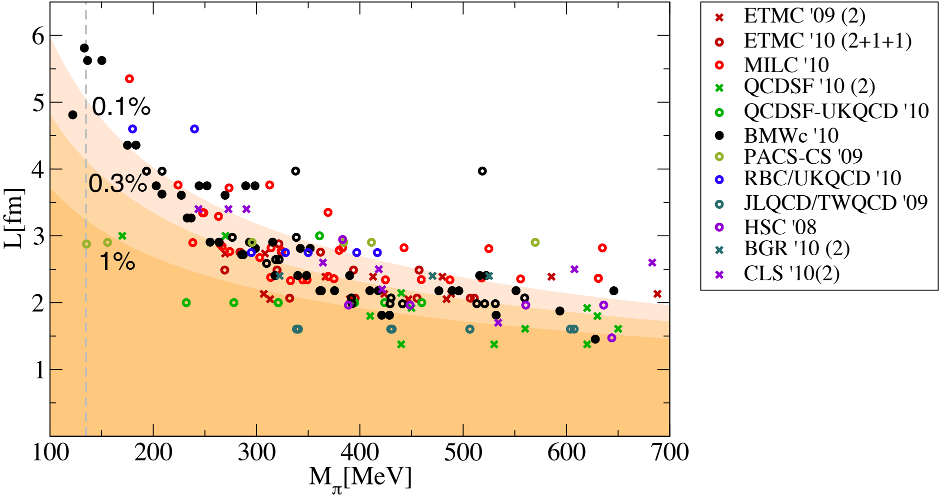
Challenge:

- Minimize and control all systematics
  - 2+1 dynamical fermion flavors
  - Physical quark masses
  - Continuum extrapolation
  - Nonperturbative renormalization (where applicable)
  - Infinite volume

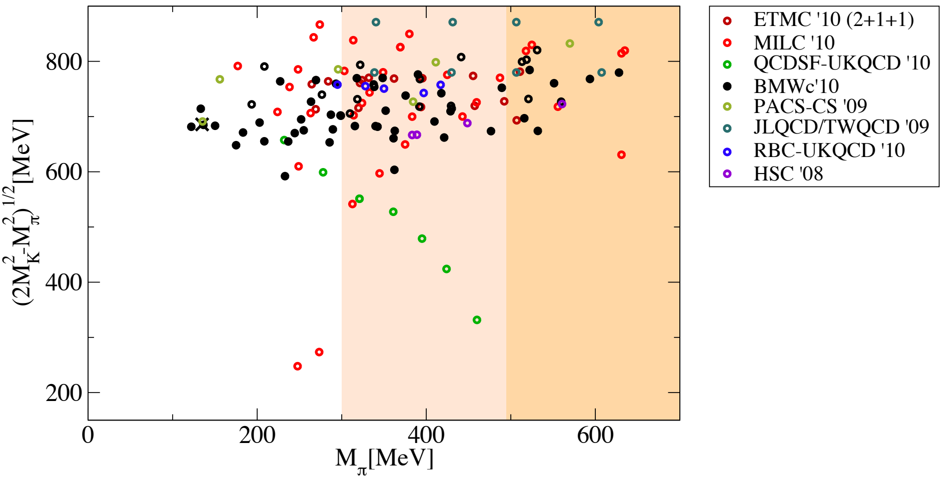
Landscape M_π vs. a



Landscape L vs. M_π



Landscape M_K vs. M_π



Action details

Goal:

- Optimize physics results per CPU time
- Conceptually clean formulation

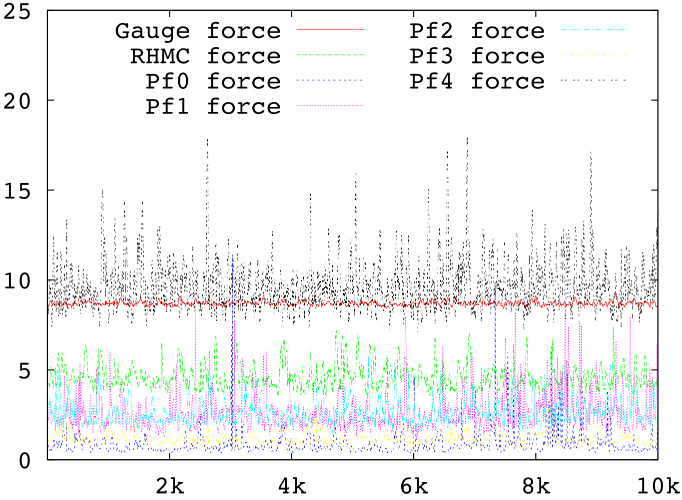
Method:

- Dynamical $2+1$ flavor, Wilson fermions at physical M_π
- 3-5 lattice spacings $0.053\text{ fm} < a < 0.125\text{ fm}$
- Tree level $O(a^2)$ improved gauge action (Lüscher, Weisz, 1985)
- Tree level $O(a)$ improved fermion action (Sheikholeslami, Wohlert, 1985)
    - Why not go beyond tree level?
        - Keeping it simple (parameter fine tuning)
        - No real improvement, UV mode suppression took care of this
    - This is a crucial advantage of our approach
- UV filtering (APE coll. 1985; Hasenfratz, Knechtli, 2001; Capitani, Durr, C.H., 2006)

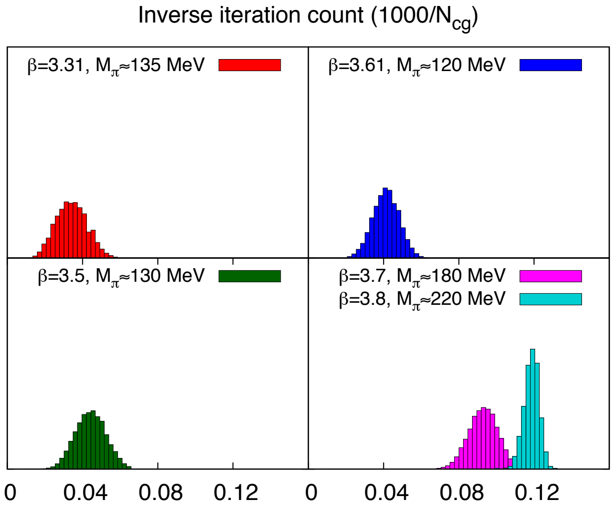
➢ Discretization effects of $O(\alpha_s a, a^2)$

✓ We include both $O(\alpha_s a)$ and $O(a^2)$ into systematic error

Algorithm stability

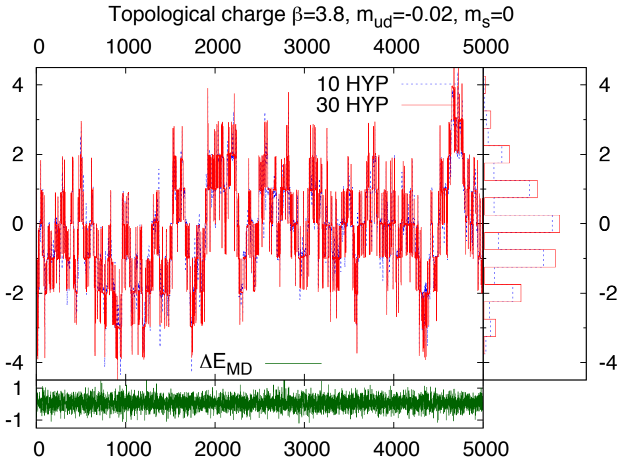


No exceptional configs



Topological sector sampling

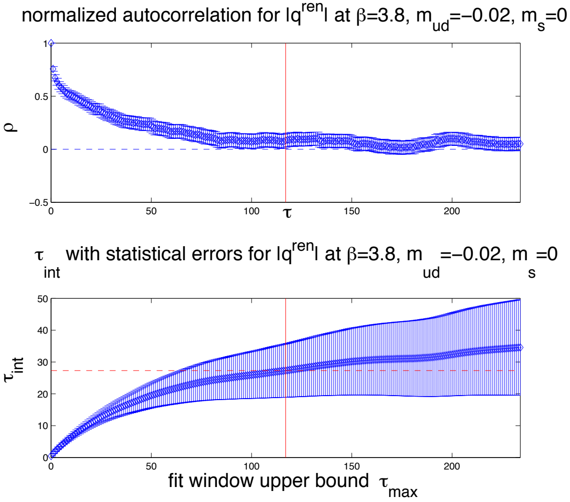
worst case



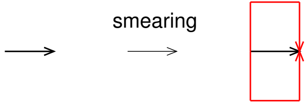
Autocorrelation time (finest lattice, small mass)

$\tau_{\text{int}} = 27.3(7.4)$

(MATLAB code from Wolff, 2004-7)



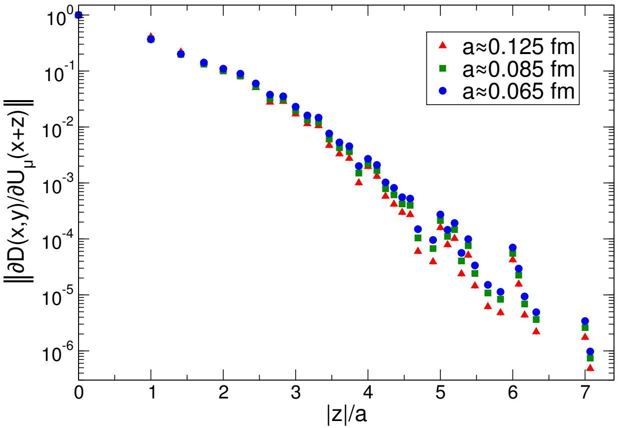
Locality properties



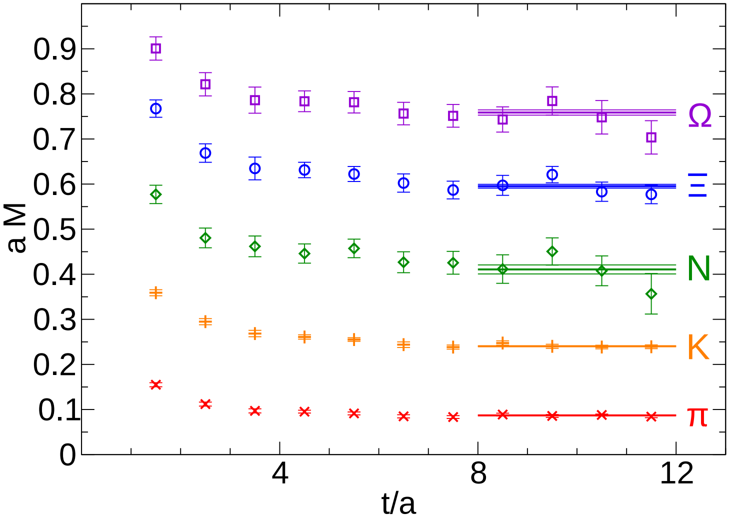
- locality in position space:
  $|D(x,y)| < \mathrm{const}\, e^{-\lambda|x-y|}$ with $\lambda = O(a^{-1})$ for all couplings.
  Our case: $D(x,y) = 0$ as soon as $|x-y| > 1$
  (despite smearing)
- locality of gauge field coupling:
  $|\delta D(x,y)/\delta A(z)| < \mathrm{const}\, e^{-\lambda|(x+y)/2-z|}$ with $\lambda = O(a^{-1})$ for all couplings.
  Our case: $\delta D(x,x)/\delta A(z) < \mathrm{const}\, e^{-\lambda|x-z|}$ with $\lambda \simeq 2.2a^{-1}$ for $2 \leq |x-z| \leq 6$

Gauge field coupling locality

6-stout case:

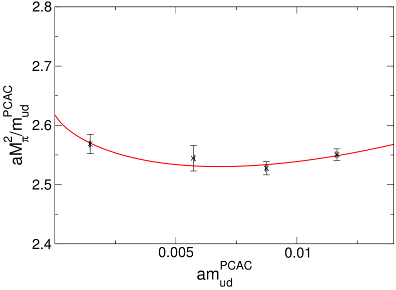


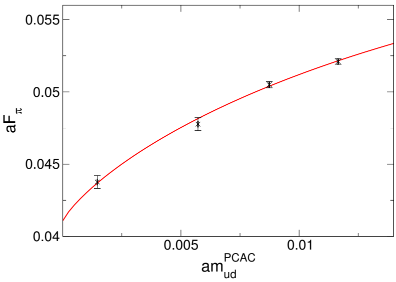
Effective masses and correlated fits



Chiral interpolation

- Simultaneous fit to NLO $SU(2)$ χPT (Gasser, Leutwyler, 1984)
- Consistent for $M_\pi \lesssim 400$ MeV





➢ We use 2 safe chiral interpolation ranges: $M_\pi < 340, 380$ MeV

➢ We use $SU(2)$ χPT and Taylor interpolation forms

Light hadron spectrum

- Goal:
  - Firmly establish (or invalidate?) QCD as the theory of strong interaction in the low energy region
- Method:
  - Post-diction of light hadron spectrum
    - Octet baryons
    - Decuplet baryons
    - Vector mesons
- Challenge:
  - Minimize and control all systematics
    - 2+1 dynamical fermion flavors
    - Physical quark masses
    - Continuum
    - Infinite volume (treatment of resonant states)

Scale setting

Goal:

- Unambiguous, precise scale setting

Method:

- We set the scale via a baryon mass
- Desirable properties:
  - experimentally well known
  - small lattice error (Octet better than Decuplet)
  - independent of light quark mass $\rightarrow$ large strange content
- Best candidates:
  - Ξ: largest strange content of the octet
  - Ω: member of the decuplet, but no light quarks

Quark mass dependence

Goal:

- Extra-/Interpolate M_X (baryon/vector meson mass) to physical point (M_π, M_K)

Method:

- Fundamental parameters: g, m_{ud}, m_s
  - Experimentally inaccessible (confinement!)
  - Must be set via 3 experimentally accessible quantities
- Use M_Ξ or M_Ω and M_π, M_K to set parameters
- Variables to parametrize M_π^2 and M_K^2 dependence of M_X:
  - Use bare masses aM_y, $y \in \{X, \pi, K\}$ and a (bootstrapped)
  - Use dimensionless ratios $r_y := \frac{M_y}{M_{\Xi/\Omega}}$ (cancellations)

We use both procedures ➛systematic error

Quark mass dependence (ctd.)

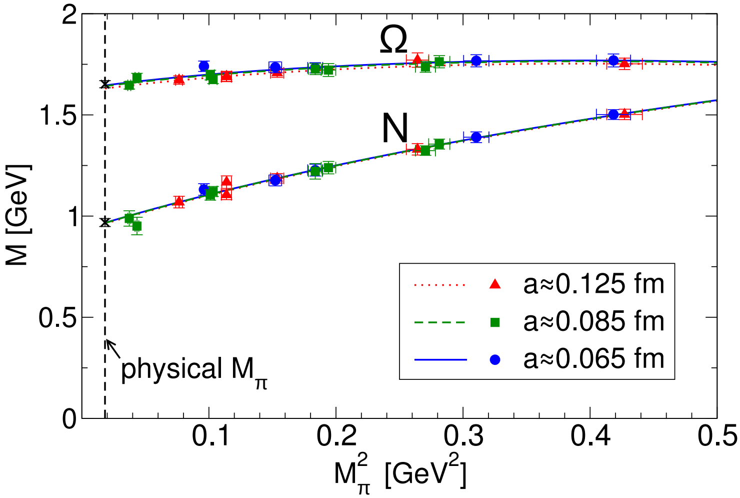
Method (ctd.):

- Parametrization: $M_X = M_X^{(0)} + \alpha M_\pi^2 + \beta M_K^2 +$ higher orders
  - Leading order sufficinet for M_K^2 dependence
  - We include higher order term in M_π^2
    - Next order χPT (around $M_\pi^2 = 0$): $\propto M_\pi^3$
    - Taylor expansion (around $M_\pi^2 \neq 0$): $\propto M_\pi^4$

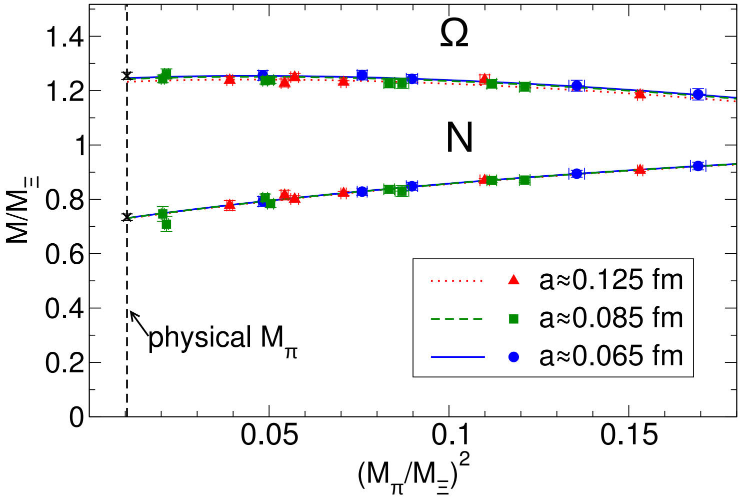
  Both procedures fine ➛systematic error
  No sensitivity to any order beyond these
- Vector mesons: higher orders not significant
- Baryons: higher orders significant
  - Restrict fit range to further estimate systematics:
    - full range, $M_\pi < 550/450$MeV

  We use all 3 ranges ➛systematic error

Chiral fit


2
1.5
1
0.5
0
0.1
0.2
0.3
0.4
0.5
M [GeV]
M_π^2 [GeV^2]
Ω
N
physical M_π
a≈0.125 fm
a≈0.085 fm
a≈0.065 fm

Chiral fit using ratios



Continuum extrapolation

Goal:

- Eliminate discretization effects

Method:

- Formally in our action: $O(\alpha_s a)$ and $O(a^2)$
- Discretization effects are tiny
  - Not possible to distinguish between $O(a)$ and $O(a^2)$

➛include both in systematic error

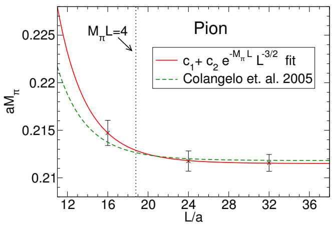
Finite volume effects from virtual pions

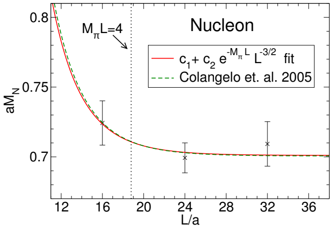
Goal:

- Eliminate virtual pion finite V effects
  - Hadrons see mirror charges
  - Exponential in lightest particle (pion) mass

Method:

- Best practice: use large V
  - Rule of thumb: $M_\pi L \gtrsim 4$
  - Leading effects $\frac{M_X(L)-M_X}{M_X} = cM_\pi^{1/2} L^{-3/2} e^{M_\pi L}$ (Colangelo et. al., 2005)





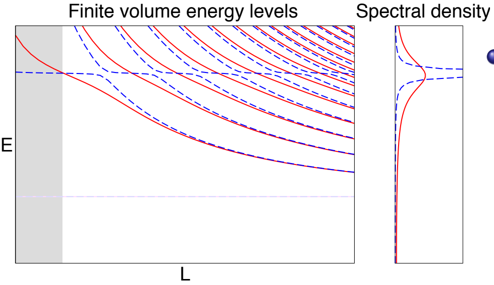
Finite volume effects in resonances

Goal:

- Eliminate spectrum distortions from resonances mixing with scattering states

Method:

- Stay in region where resonance is ground state
  - Otherwise no sensitivity to resonance mass in ground state



- Treatment as scattering problem

  (Lüscher, 1985-1991)
  - Parameters: mass and coupling (width)
  - Alternative approaches suggested

Systematic uncertainties

Goal:

- Accurately estimate total systematic error

Method:

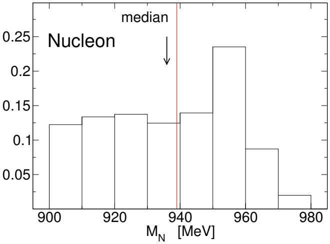
- We account for all the above mentioned effects
- When there are a number of sensible ways to proceed, we take them: Complete analysis for each of
  - 18 fit range combinations
  - ratio/nonratio fits (r_X resp. M_X)
  - $O(a)$ and $O(a^2)$ discretization terms
  - NLO χPT M_π^3 and Taylor M_π^4 chiral fit
  - 3 χ fit ranges for baryons: $M_\pi < 650/550/450$ MeV

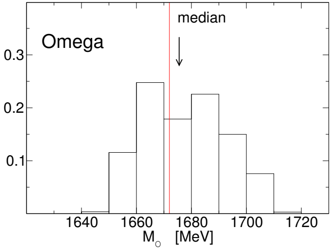
resulting in 432 (144) predictions for each baryon (vector meson) mass with each 2000 bootstrap samples for each Ξ and Ω scale setting

Systematic uncertainties II

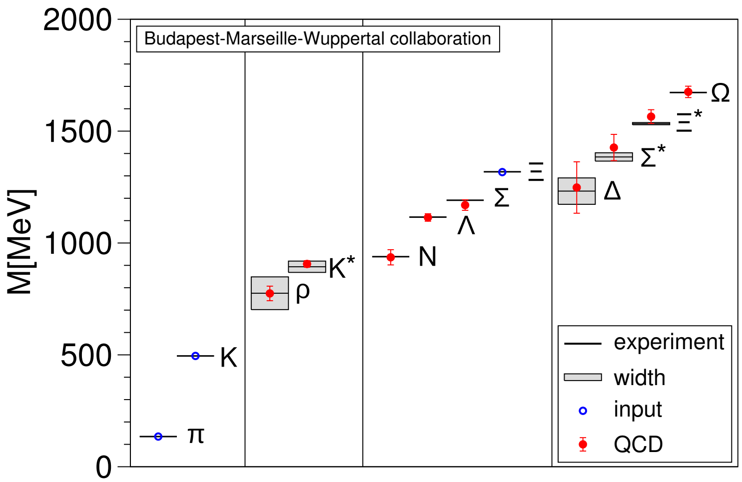
Method (ctd.):

- Weigh each of the 432 (144) central values by fit quality Q
  - Median of this distribution ➛final result
  - Central 68% ➛systematic error
- Statistical error from bootstrap of the medians





The light hadron spectrum



Pseudoscalar decay constant ratio

- Goal:
  - Check first row unitarity of CKM matrix
- Method:
  - Compute F_K/F_π
  - Perturbative relation to $|V_{us}|^2/|V_{ud}|^2$ with 0.4% accuracy
- Challenge:
  - Minimize and control all systematics
    - 2+1 dynamical fermion flavors
    - Physical quark masses
    - Continuum
    - Infinite volume

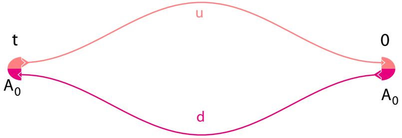
Observable

With the axial vector current

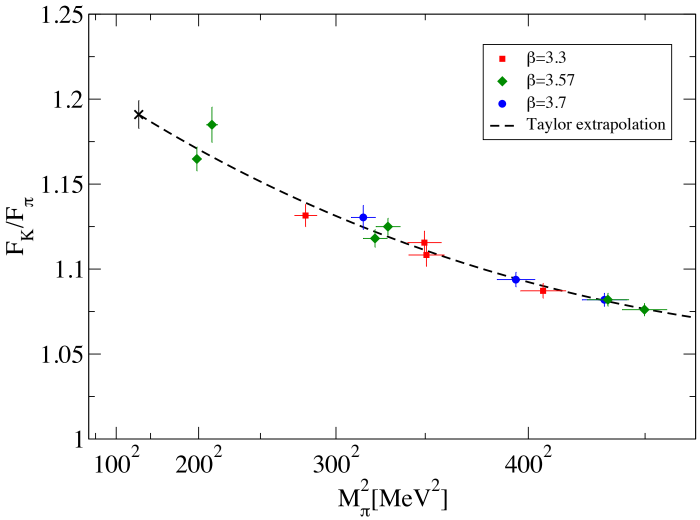
$$A_\mu(t) = \sum_{\vec{x}} \left(\bar{\Psi}^d \gamma_\mu \gamma_5 \Psi^u \right)(\vec{x}, t)$$

one obtains

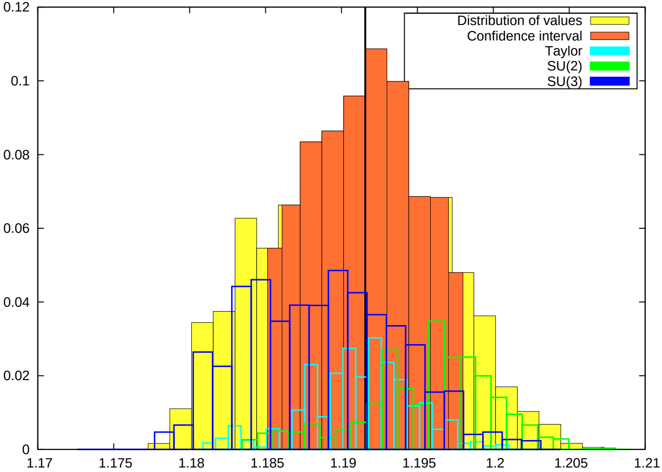
$$\langle A_0^\dagger(t) A_0(0) \rangle \xrightarrow{t\to\infty} \frac{|\langle \pi | A_0 | 0 \rangle|^2}{2M_\pi} e^{-M_\pi t} = \frac{M_\pi^2 {F_\pi^{\text{bare}}}^2}{2M_\pi} e^{-M_\pi t}$$



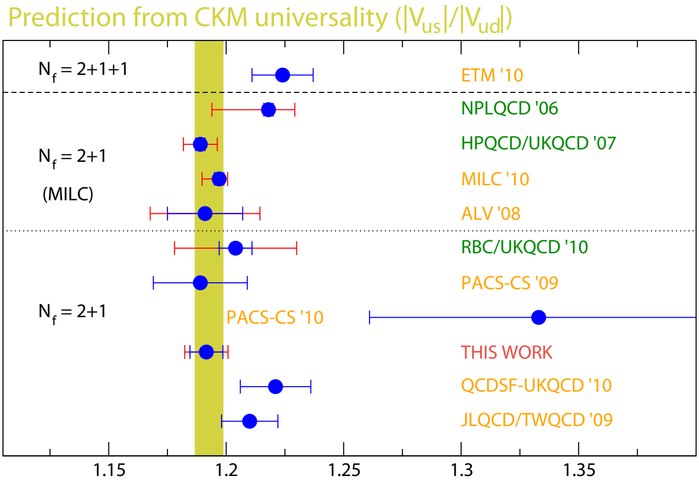
Chiral extrapolation



Errors


Distribution of values
Confidence interval
Taylor
SU(2)
SU(3)
0.12
0.1
0.08
0.06
0.04
0.02
0
1.17
1.175
1.18
1.185
1.19
1.195
1.2
1.205
1.21

Comparison


Prediction from CKM universality (|V_us|/|V_ud|)
N_f = 2+1+1
ETM '10
NPLQCD '06
HPQCD/UKQCD '07
N_f = 2+1
(MILC)
MILC '10
ALV '08
RBC/UKQCD '10
PACS-CS '09
N_f = 2+1
PACS-CS '10
THIS WORK
QCDSF-UKQCD '10
JLQCD/TWQCD '09
1.15
1.2
1.25
1.3
1.35

Strategy outline

Goal:

- Compute light quark masses ab initio

Relevance:

- Fundamental SM parameters
- Stability of matter depends on their values
- Not obtainable perturbatively

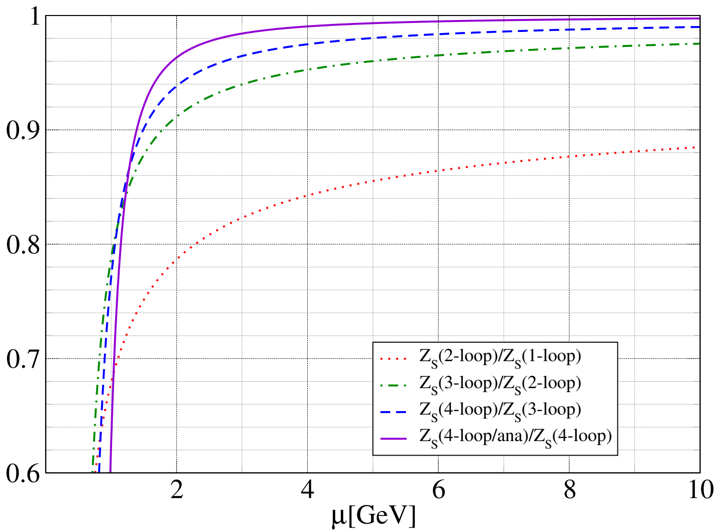
Challenge:

- Minimize and control all systematics
  - 2+1 dynamical fermion flavors
  - Physical quark masses
  - Continuum extrapolation
  - Nonperturbative renormalization
  - Infinite volume

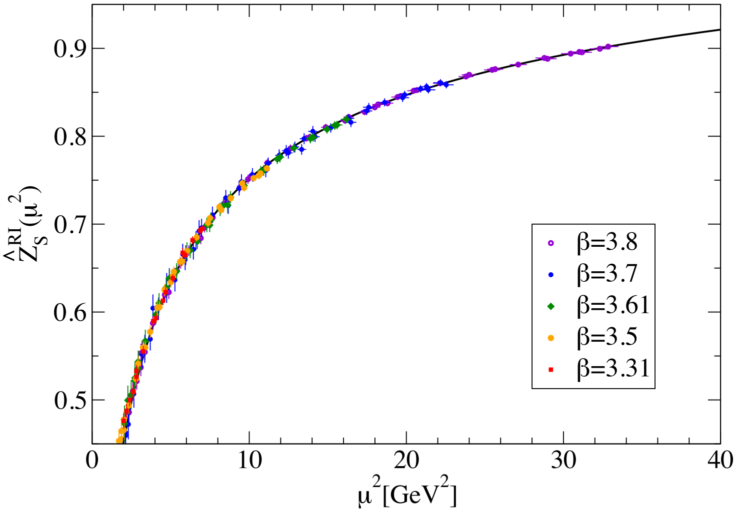
Renormalization strategy

- Goal:
  - Full nonperturbative renormalization
  - Optional accurate conversion to perturbative scheme
- Method:
  - We use RI-MOM scheme (Martinelli et. al., 1993)
    - $O(a)$ correction (Maillart, Niedermayer, 2008)
  - Compute m_q at low scale $\mu \ll 2\pi/a \sim 11 - 24$ GeV
    - $\mu = 2.1 GeV$
    - $\mu = 1.3 GeV$
  - Do continuum non-perturbative running to high scale $\mu' \gg \Lambda_{QCD}$
  - Further conversion in 4-loop PT

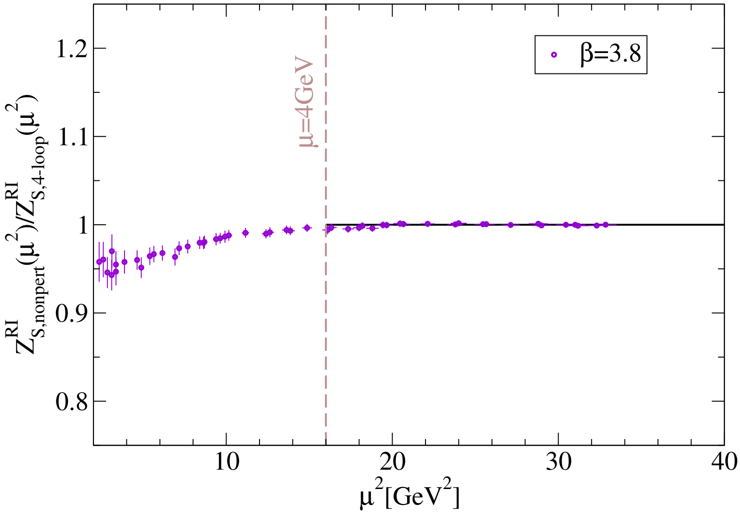
Desired scale in RI-MOM scheme



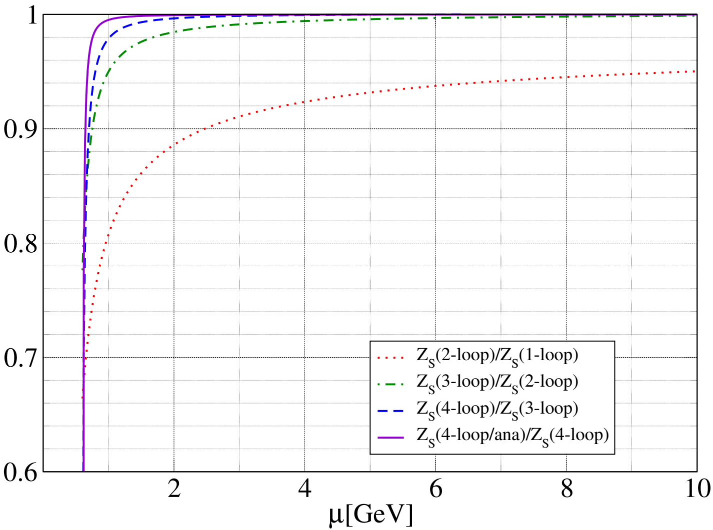
Nonperturbative running



Reaching the perturbative regime



Optional conversion to $\overline{\text{MS}}$



Quark mass definitions

- Lagrangian mass m^{bare}
- $m^{\text{ren}} = \frac{1}{Z_S}(m^{\text{bare}} - m^{\text{bare}}_{\text{crit}})$

- m^{PCAC} from $\frac{\langle \partial_0 A_0 P \rangle}{\langle P(t) P(0) \rangle}$
- $m^{\text{ren}} = \frac{Z_A}{Z_P} m^{\text{PCAC}}$

Better use

- $d = m_s^{\text{bare}} - m_{ud}^{\text{bare}}$
- $d^{\text{ren}} = \frac{1}{Z_S} d$

- $r = m_s^{\text{PCAC}} / m_{ud}^{\text{PCAC}}$
- $r^{\text{ren}} = r$

and reconstruct

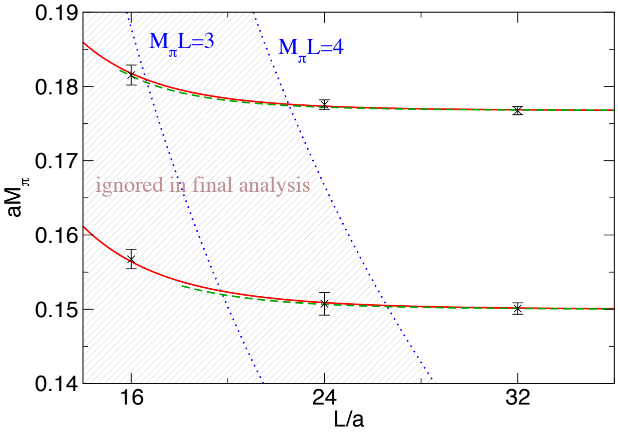
- $m_s^{\text{ren}} = \frac{1}{Z_S} \frac{rd}{r-1}$
- $m_{ud}^{\text{ren}} = \frac{1}{Z_S} \frac{d}{r-1}$

✓ No additive mass renormalization and ambiguity in m_{crit}

✓ Only Z_S multiplicative renormalization (no pion poles)

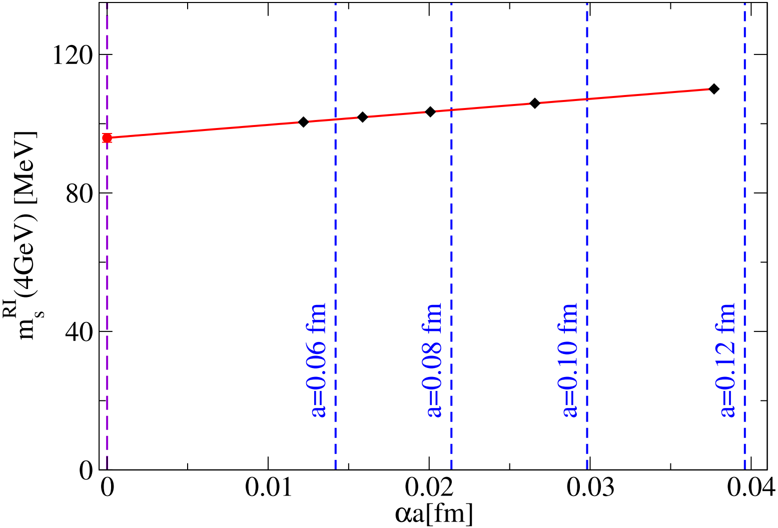
☞ Works with $O(a)$ improvement (we use this)

Tiny finite volume effects

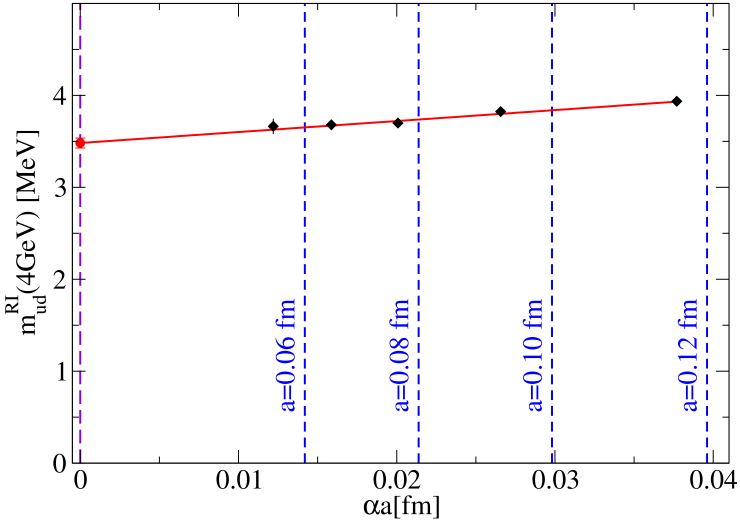


- FV effects tiny
- Dedicated FV runs
- Perfect agreement with FV χPT (Colangelo et. al. 2005)

Strange quark mass



Light quark masses



Individual m_u and m_d

- Goal:
  - Compute m_u and m_d separately
- Method:
  - Need QED and isospin breaking effects in principle
  - Alternative: use dispersive input -Q from $\eta \to \pi\pi\pi$

    $$Q^2 = \frac{1}{2}\left(\frac{m_s}{m_{ud}}\right)^2 \frac{m_d - m_u}{m_{ud}}$$

  ✓ Transform precise m_s/m_{ud} into $(m_d - m_u)/m_{ud}$
  - We use the conservative $Q = 22.3(8)$ (Leutwyler, 2009)

Systematic error treatment

- Goal:
  - Reliably estimate total systematic error
- Method:
  - 288 full analyses (2000 bootstrap on each)
    - 2 plateaux regions
    - 2 continuum forms: $O(\alpha_s a)$, $O(a^2)$
    - 3 chiral forms: $2 \times SU(2)$, Taylor
    - 2 chiral ranges: $M_\pi < 340, 380$ MeV
    - 3 renormalization matching procedures
    - 2 NP continuum running forms
    - 2 scale setting procedures
  - All analyses weighted by fit quality
    - Mean gives final result
    - Stdev gives systematic error
  - Statistical error from 2000 bootstrap samples

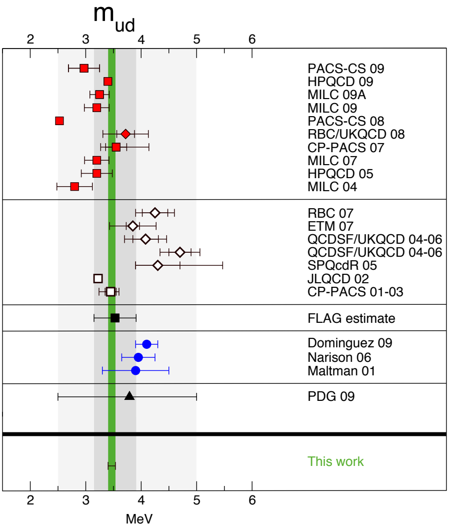
Final result

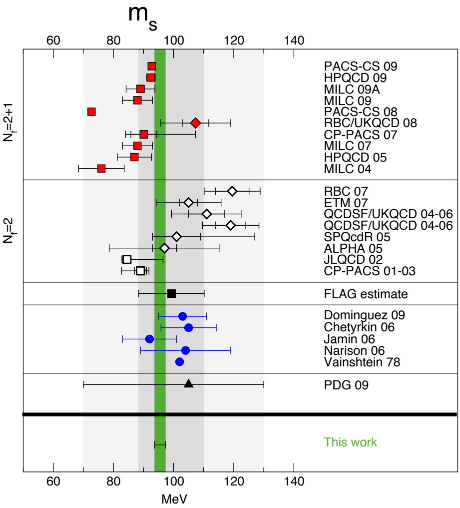
	RI @ 4 GeV	RGI	$\overline{\text{MS}}$ @ 2 GeV
m_s	96.4(1.1)(1.5)	127.3(1.5)(1.9)	95.5(1.1)(1.5)
m_{ud}	3.503(48)(49)	4.624(63)(64)	3.469(47)(48)
m_u	2.17(04)(10)	2.86(05)(13)	2.15(03)(10)
m_d	4.84(07)(12)	6.39(09)(15)	4.79(07)(12)

Additional consistency checks:

- ✓ Use m^{PCAC} only, no ratio-difference method
  ☞compatible, slightly larger error
- ✓ Unweighted final result and systematic error
  ☞negligible impact
- ✓ Additional Continuum, chiral and FV terms
  ☞all compatible with 0

Comparison


m_{ud}
PACS-CS 09
HPQCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPQCD 05
MILC 04
RBC 07
ETM 07
QCDSF/UKQCD 04-06
QCDSF/UKQCD 04-06
SPQcdR 05
JLQCD 02
CP-PACS 01-03
FLAG estimate
Dominguez 09
Narison 06
Maltman 01
PDG 09
This work
2 3 4 5 6
MeV


m_s
N_f=2+1
N_f=2
PACS-CS 09
HPQCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPQCD 05
MILC 04
RBC 07
ETM 07
QCDSF/UKQCD 04-06
QCDSF/UKQCD 04-06
SPQcdR 05
ALPHA 05
JLQCD 02
CP-PACS 01-03
FLAG estimate
Dominguez 09
Chetyrkin 06
Jamin 06
Narison 06
Vainshtein 78
PDG 09
This work
60 80 100 120 140
MeV

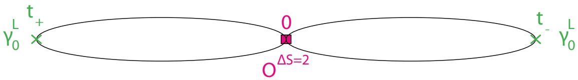
Standard model neutral K mixing

- Goal:
  - Check SM CP violation in neutral K system
- Method:
  - Compute effective weak matrix element
  - Relate kaon CP violation to CKM phase
- Challenge:
  - Minimize and control all systematics
    - 2+1 dynamical fermion flavors
    - Physical quark masses
    - Mixing of unphysical operators
    - Continuum
    - Infinite volume

Observable

Matrix element of an effective weak operator (e.g. $\langle K^\dagger | O | K \rangle$):

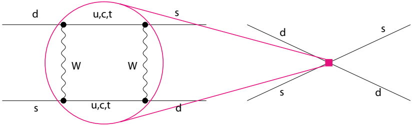
$$\langle J_0^{L\dagger}(t_+) O(0) J_0^L(t_-) \rangle \overset{t_\pm \to \pm\infty}{\longrightarrow} \frac{|\langle K | J_0^L | 0 \rangle|^2}{(2M_K)^2} \langle K^\dagger | O | K \rangle e^{-M_K(t_+ - t_-)}$$



where

$$J_0^L = [\bar{s}d]_{V-A} = \bar{s}\gamma_0(1-\gamma_5)d$$

$$O_{\Delta S=2} = [\bar{s}d]_{V-A}[\bar{s}d]_{V-A}$$

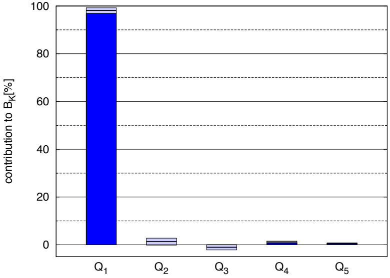


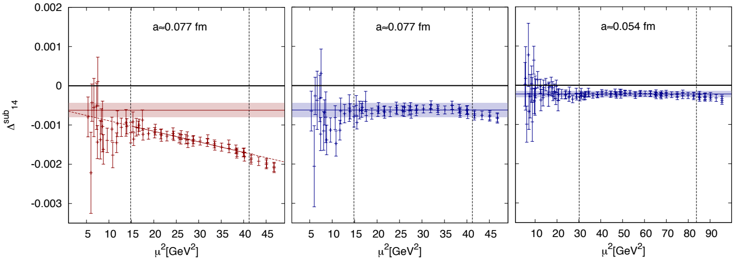
Norm from:

$$\langle J_0^{L\dagger}(t) J_0^L(0) \rangle \overset{t \to \infty}{\longrightarrow} \frac{|\langle K | J_0^L | 0 \rangle|^2}{2M_K} e^{-M_K t}$$

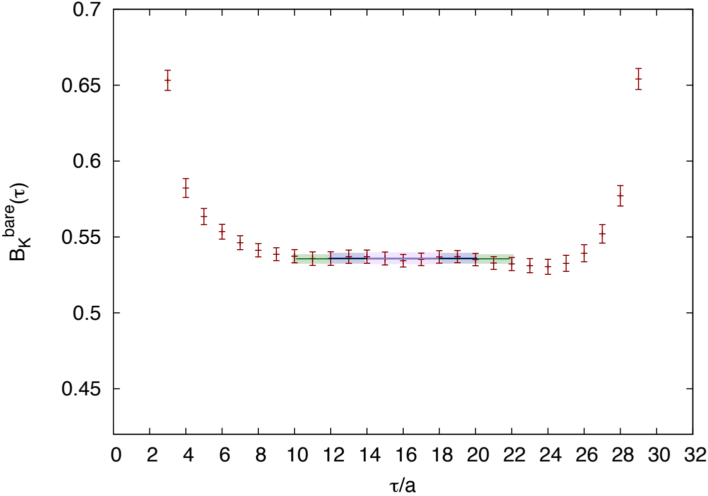
Unphysical operator mixing

- χSB induces mixing with 4 unphysical operators
- Mixing terms chirally enhanced
- ✓ Small even below physical m_π
- ✓ Good chirality of our action

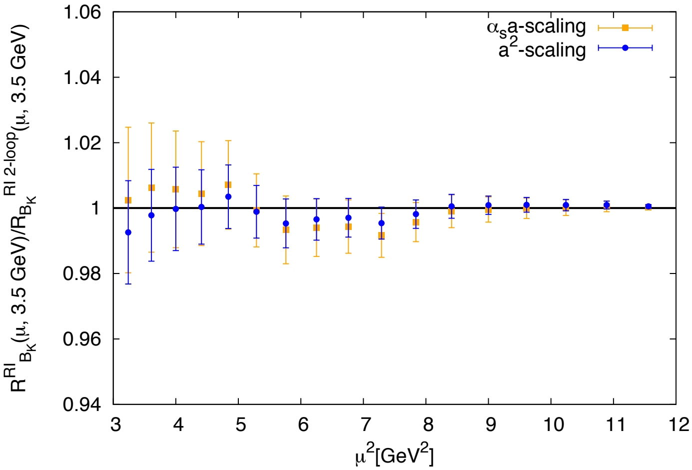




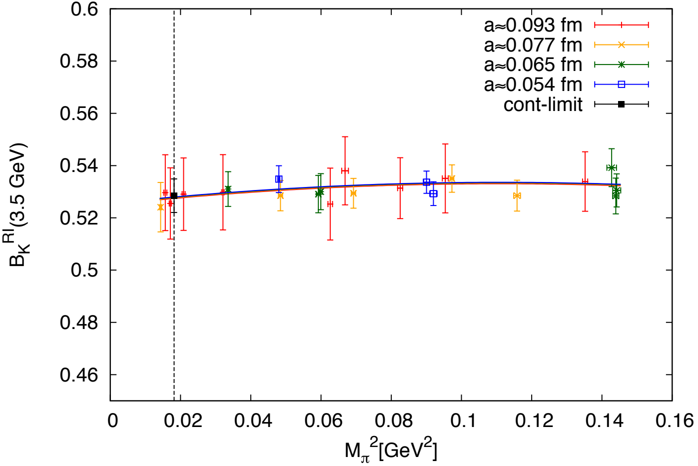
Signal


0.7
0.65
0.6
0.55
0.5
0.45
$B_K^{bare}(\tau)$
0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32
τ/a

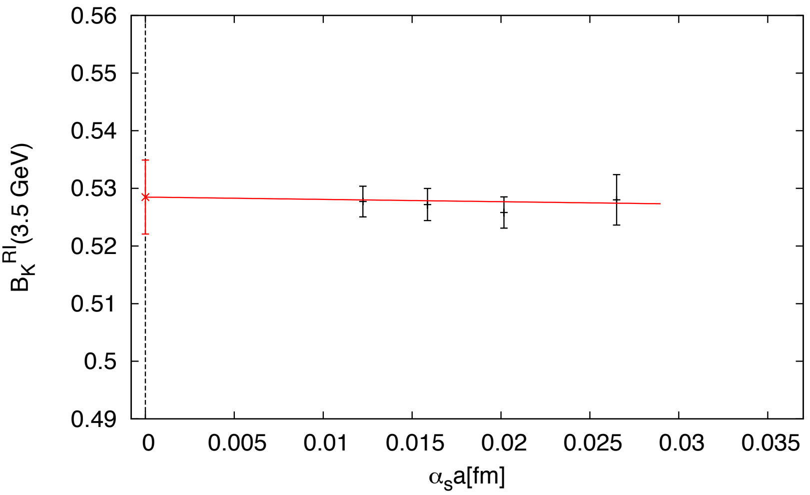
Running


α_sa-scaling
a^2-scaling
$R^{RI}_{B_K}(\mu, 3.5\text{ GeV})/R^{RI\ 2\text{-loop}}_{B_K}(\mu, 3.5\text{ GeV})$
$\mu^2[\text{GeV}^2]$
1.06
1.04
1.02
1
0.98
0.96
0.94
3
4
5
6
7
8
9
10
11
12

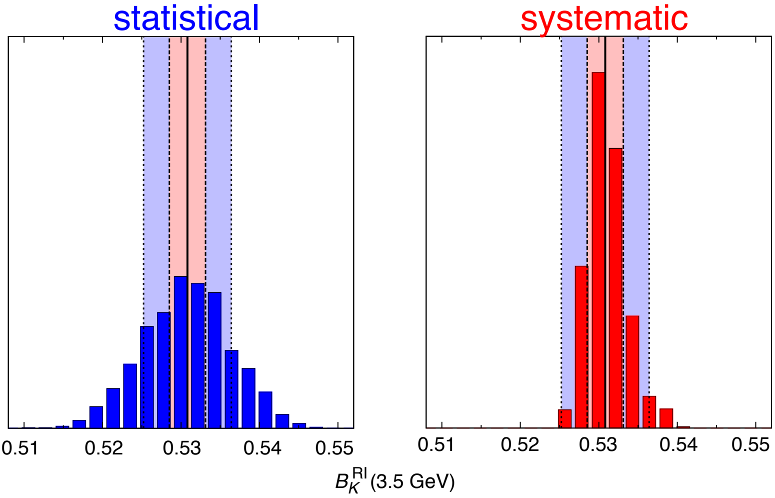
Physical point



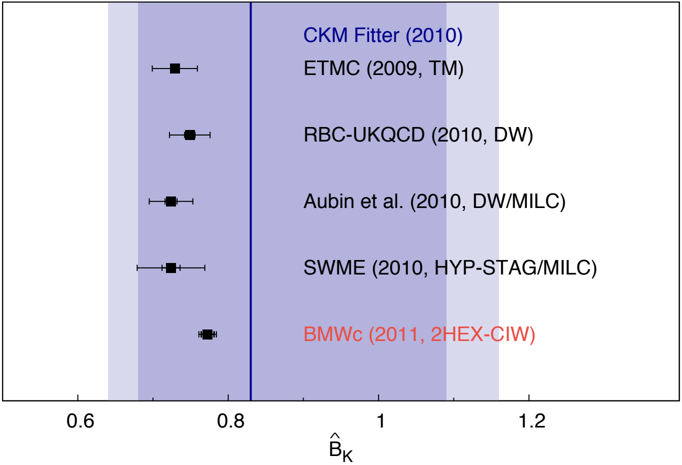
Continuum extrapolation

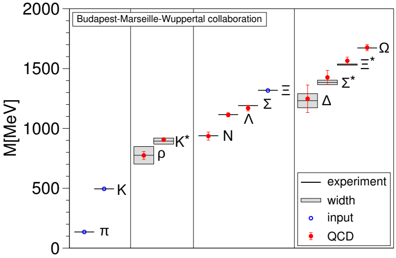


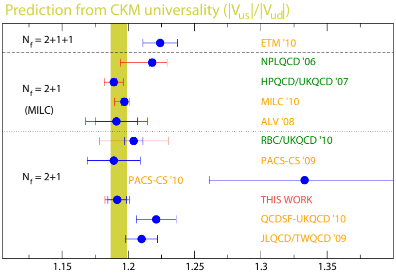
Errors

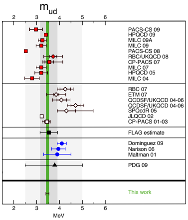

statistical
systematic
0.51
0.52
0.53
0.54
0.55
0.51
0.52
0.53
0.54
0.55
$B_K^{RI}(3.5\ \text{GeV})$

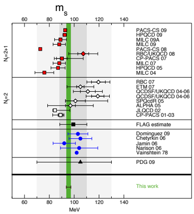
Comparison

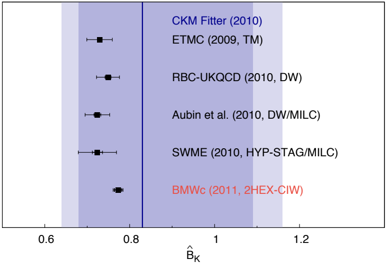

CKM Fitter (2010)
ETMC (2009, TM)
RBC-UKQCD (2010, DW)
Aubin et al. (2010, DW/MILC)
SWME (2010, HYP-STAG/MILC)
BMWc (2011, 2HEX-CIW)
0.6
0.8
1
1.2
$\hat{B}_K$


Budapest-Marseille-Wuppertal collaboration
M[MeV]
2000
1500
1000
500
0
π
K
ρ
K*
N
Λ
Σ
Ξ
Δ
Σ*
Ξ*
Ω
experiment
width
input
QCD


Prediction from CKM universality (|Vus|/|Vud|)
Nf = 2+1+1
Nf = 2+1
(MILC)
Nf = 2+1
ETM '10
NPLQCD '06
HPQCD/UKQCD '07
MILC '10
ALV '08
RBC/UKQCD '10
PACS-CS '09
PACS-CS '10
THIS WORK
QCDSF-UKQCD '10
JLQCD/TWQCD '09
1.15
1.2
1.25
1.3
1.35

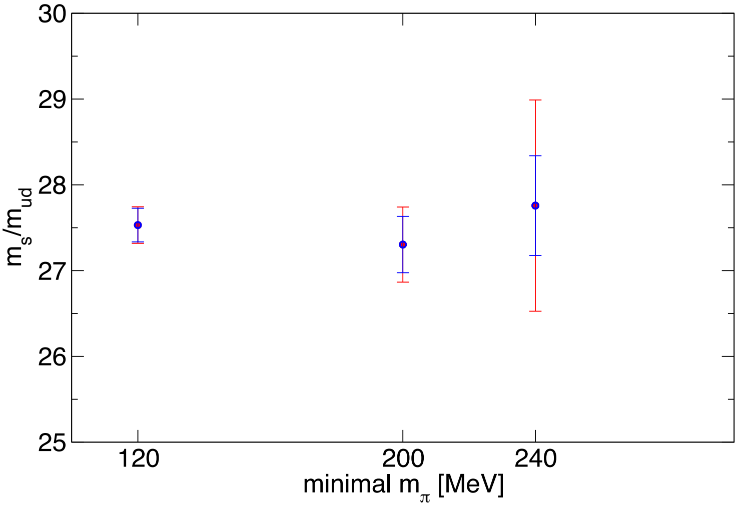

mud
2
3
4
5
6
PACS-CS 09
HPQCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPQCD 05
MILC 04
RBC 07
ETM 07
QCDSF/UKQCD 04-06
QCDSF/UKQCD 04-06
SPQcdR 05
JLQCD 02
CP-PACS 01-03
FLAG estimate
Dominguez 09
Narison 06
Maltman 01
PDG 09
This work
MeV


ms
60
80
100
120
140
Nf=2+1
Nf=2
PACS-CS 09
HPQCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPQCD 05
MILC 04
RBC 07
ETM 07
QCDSF/UKQCD 04-06
QCDSF/UKQCD 04-06
SPQcdR 05
ALPHA 05
JLQCD 02
CP-PACS 01-03
FLAG estimate
Dominguez 09
Chetyrkin 06
Jamin 06
Narison 06
Vainshtein 78
PDG 09
This work
MeV

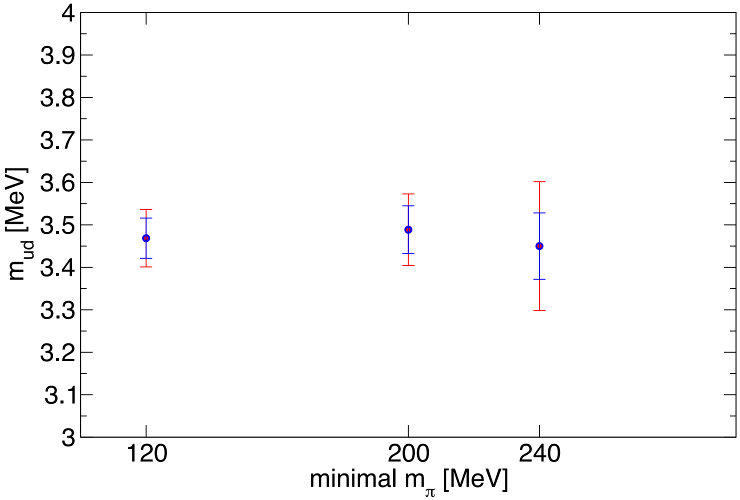

CKM Fitter (2010)
ETMC (2009, TM)
RBC-UKQCD (2010, DW)
Aubin et al. (2010, DW/MILC)
SWME (2010, HYP-STAG/MILC)
BMWc (2011, 2HEX-CIW)
0.6
0.8
1
1.2
B̂K

THE END

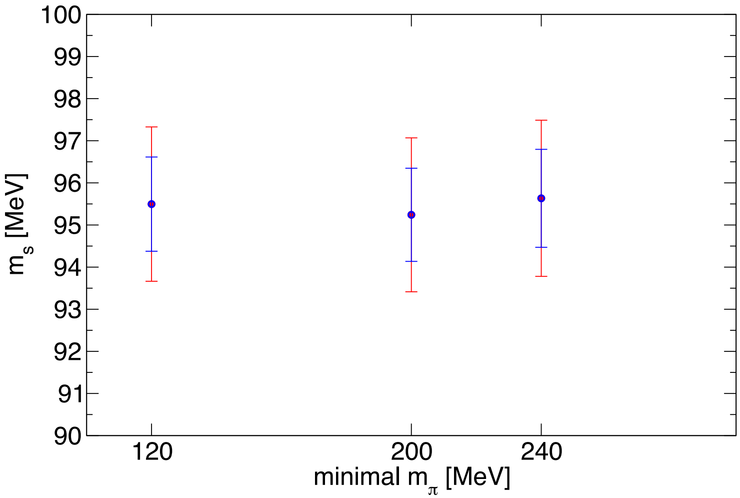
Chiral cuts



Chiral cuts



Chiral cuts



100
99
98
97
96
95
94
93
92
91
90
m_s [MeV]
120
200
240
minimal m_π [MeV]

Error budget

	cen. val.	σ_{stat}	σ_{syst}
m_{ud}	3.503	0.048	0.049
m_{s}	96.43	1.13	1.47
$m_{\mathrm{s}}/m_{\mathrm{ud}}$	27.531	0.196	0.083

Relative error contributions

plateau	scale set	fit form	mass cut	renorm.	cont.
0.330	0.034	0.030	0.157	0.080	0.926
0.207	0.005	0.031	0.085	0.085	0.970
0.513	0.200	0.023	0.320	—	0.771