Solving QCD . . . numerically

Lattice QCD at the physical point

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Motivation

Solve the low energy dynamics of QCD

- Verify that QCD is theory of strong interaction at low energies
  $\leftrightarrow$ verify the validity of the computational framework
  - $\rightarrow$ light hadron spectrum
  - $\rightarrow$ hadron interactions
  - $\rightarrow$ ...
- Fix fundamental parameters and help search for new physics
  - $\rightarrow$ m_u, m_d, m_s, ...
  - $\rightarrow$ $\langle N|m_q\bar{q}q|N\rangle$, $q = u, d, s$ for dark matter
  - $\rightarrow$ $F_K/F_\pi \leftrightarrow \frac{G_q}{G_\mu}\left[|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2\right] = 1$?
  - $\rightarrow$ $B_K \leftrightarrow$ consistency of CPV in K and B decays ?
  - $\rightarrow$ ...
- Make predictions in nuclear physics?

Introduction

Tool

$\rightarrow$ *ab initio* QCD calculations on the lattice

Challenge

- Minimize and control all systematics
  - ☞ compute hugely expensive fermion determinant
  - ☞ fight fast increasing cost of simulations as:
    - $m_{ud} \searrow m_{ud}^{\mathrm{ph}} \Rightarrow$ reach physical mass point in controlled way
    - $a \searrow 0 \Rightarrow$ controlled continuum extrapolation
    - $L \rightarrow \infty \Rightarrow$ controlled infinite volume extrapolation
  - ☞ nonperturbative renormalization
    $\Rightarrow$ eliminate all perturbative uncertainties

$\Rightarrow$ true nonperturbative QCD predictions

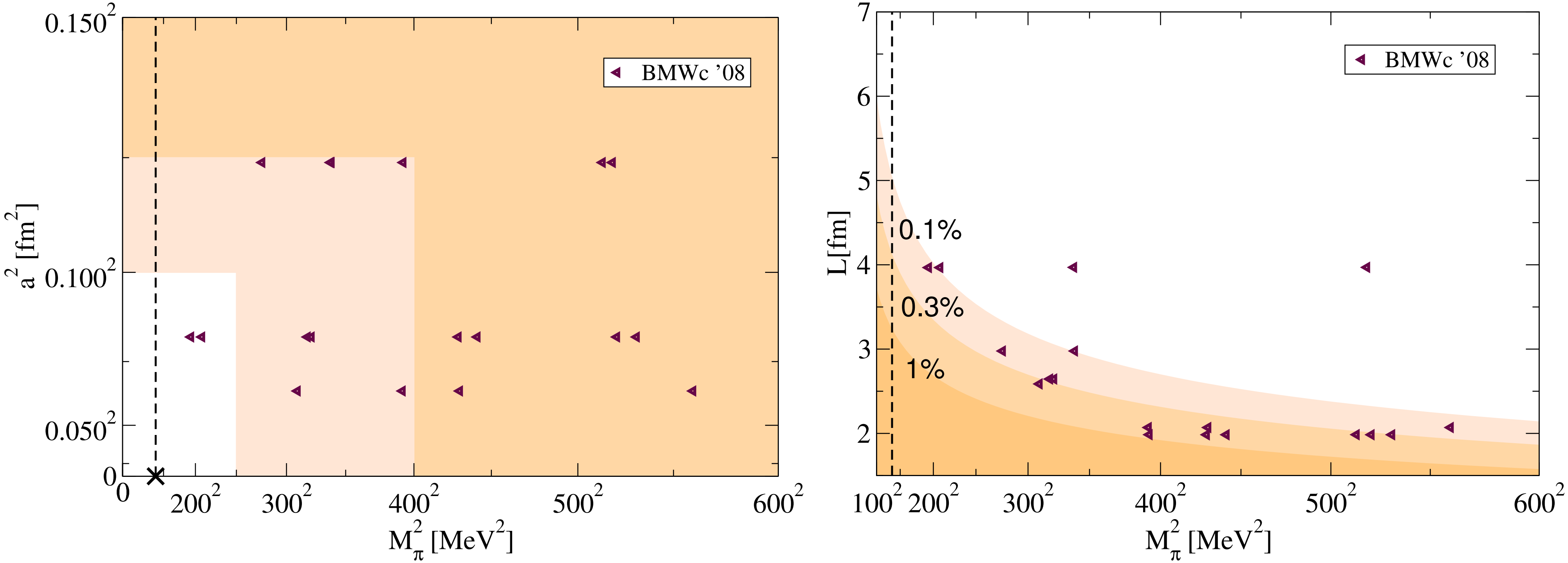
The calculation that I've been dreaming of doing

- $N_f = 2 + 1$ simulations to include u, d and s sea quark effects
- Simulations all the way down to $M_\pi \lesssim 135\,\mathrm{MeV}$ to allow small interpolation to physical mass point
- Large $L \gtrsim 5\,\mathrm{fm}$ to have sub-percent finite V errors
- At least three $a \lesssim 0.1\,\mathrm{fm}$ for controlled continuum limit
- Reliable determination of the scale w/ a well measured physical observable
- Unitary, local gauge and fermion actions
- Full nonperturbative renormalization and continuum extrapolated running if necessary
- Complete analysis of systematic uncertainties

Dürr et al (BMWc) Science 322 '08, PRD79 '09

20 large scale $N_f = 2+1$ Wilson fermion simulations

$M_\pi \gtrsim 190\,\mathrm{MeV} \qquad a \approx 0.065, 0.085, 0.125\,\mathrm{fm} \qquad L \to 4\ fm$



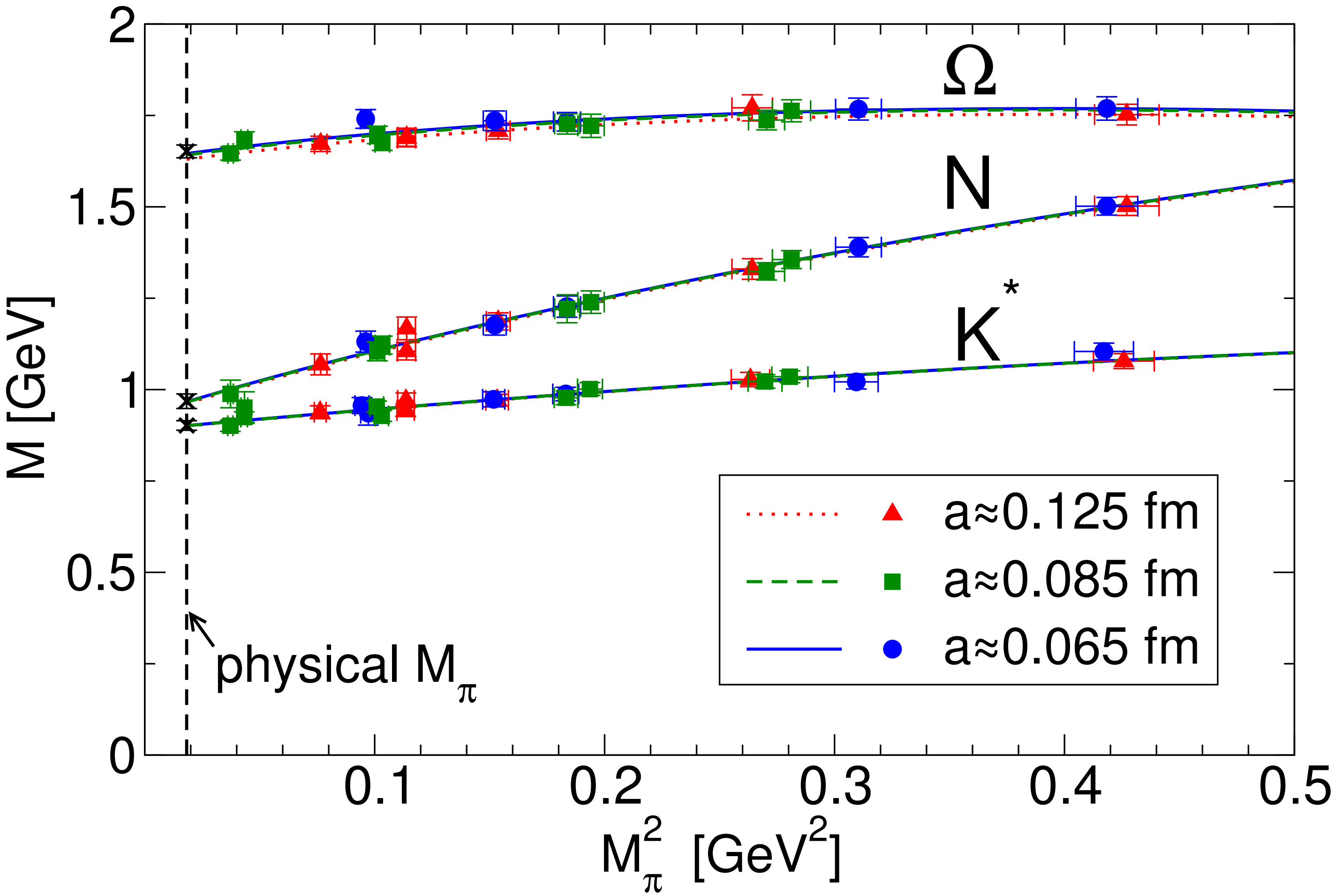
Good enough for *ab initio* calculation of light hadron masses

Computation of light hadron masses: motivations

Dürr et al (BMWc) Science 322 '08

- $>$ 99% of mass of visible universe is in the form of p & n
- Only <5% comes from mass of u and d constituents
- Important to verify that asymptotically free QCD generates this mass deficit in a way consistent w/ experiment
- Validate lattice QCD tools used
  $\Rightarrow$ reliable predictions
- Want QCD *not* lattice QCD results
  $\Rightarrow$ all necessary limits must be taken cleanly

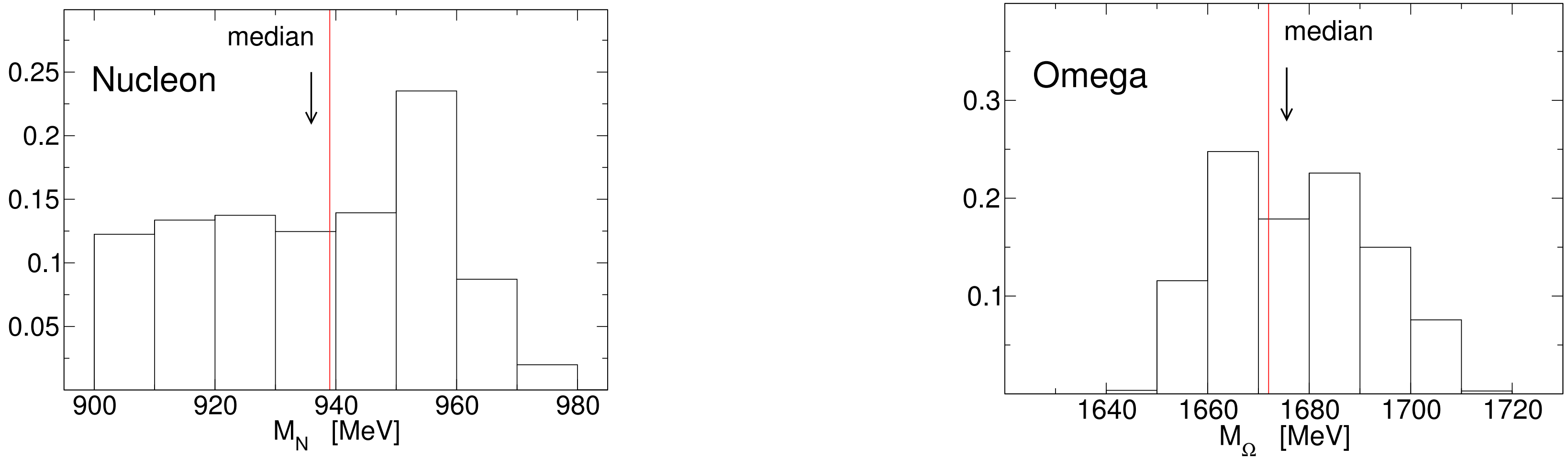
Example combined mass and continuum extrapolation



Extrapolated results very close to lightest points/small *a*-dependence
$\Rightarrow$ extrapolations fully controlled

Systematic and statistical error estimate

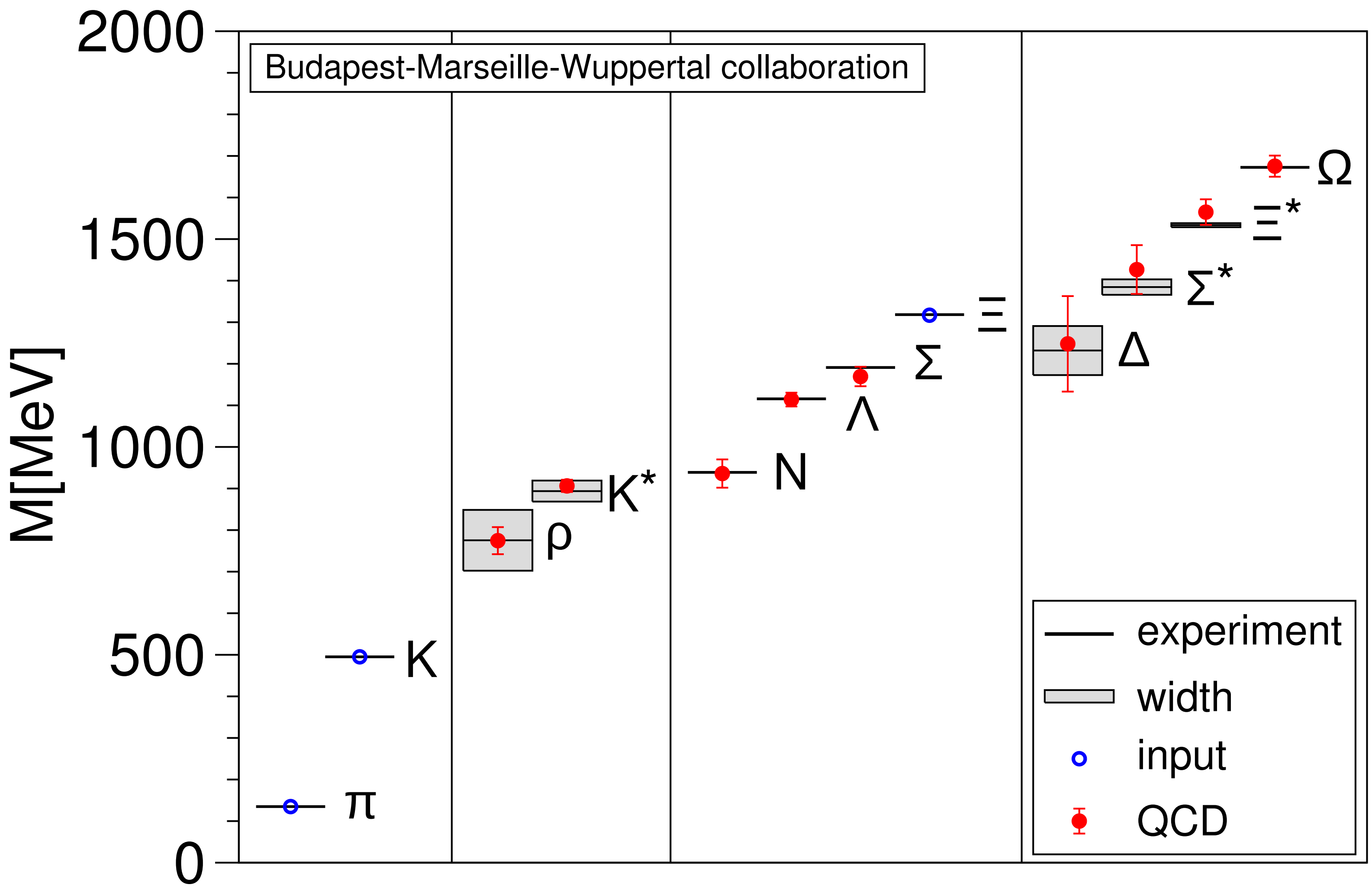
- Correct treatment of resonances (Lüscher, '85-'91)
- 432 distinct analyses for each hadron mass corresponding to different choices for: $a \searrow 0$, $M_\pi \searrow 135\,\mathrm{MeV}$, $L \nearrow \infty$, ...
- Weigh each one by fit quality $\to$ systematic error distribution
- repeat for 2000 bootstrap samples



- Median $\to$ central value
- Central 68% CI $\to$ systematic error

- Central 68% CI of bootstrap distribution of medians $\to$ statistical error

Postdiction of the light hadron masses

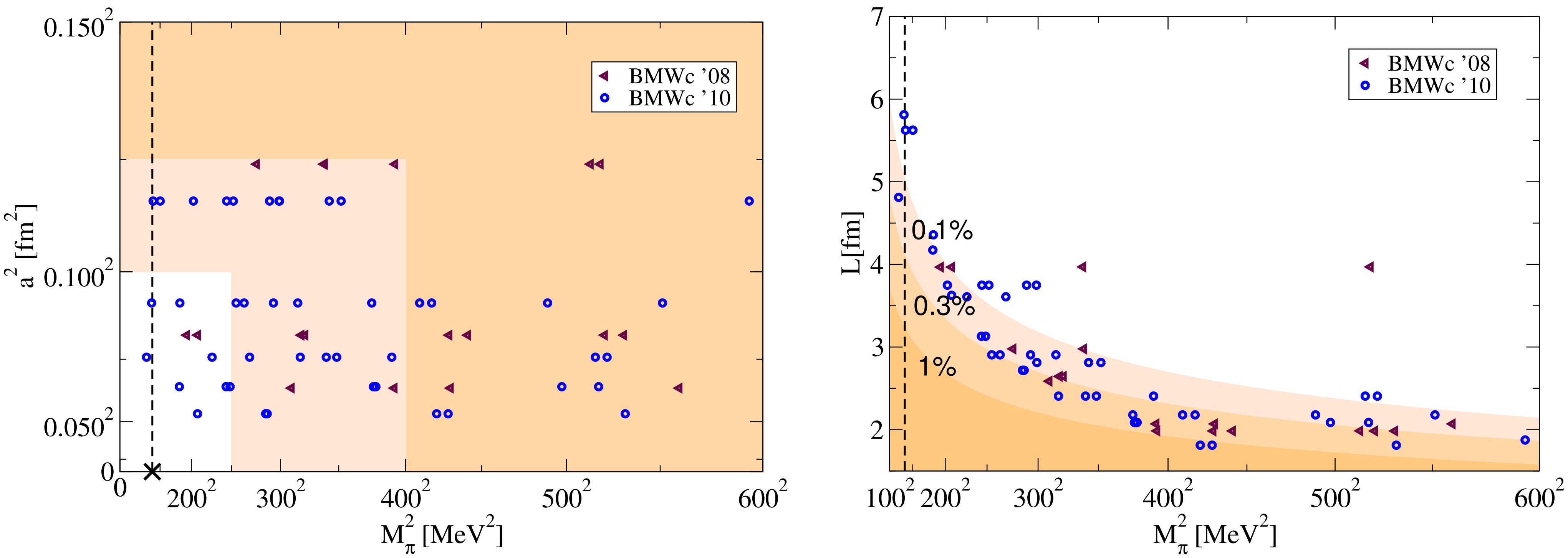


(Partial calculations by MILC '04-'09, RBC-UKQCD '07, Del Debbio et al '07, JLQCD '07, QCDSF '07-'09, Walker-Loud et al '08, PACS-CS '08-'10, ETM '09, Gattringer et al '09, . . .)

Dürr et al (BMWc) arXiv:1011.2403, arXiv:1011.2711

47 large scale $N_f = 2 + 1$ Wilson fermion simulations

$M_\pi \gtrsim 120\,\mathrm{MeV}$ $\quad$ $5a$'s $\approx 0.054 \div 0.116\,\mathrm{fm}$ $\quad$ $L \to 6\ fm$



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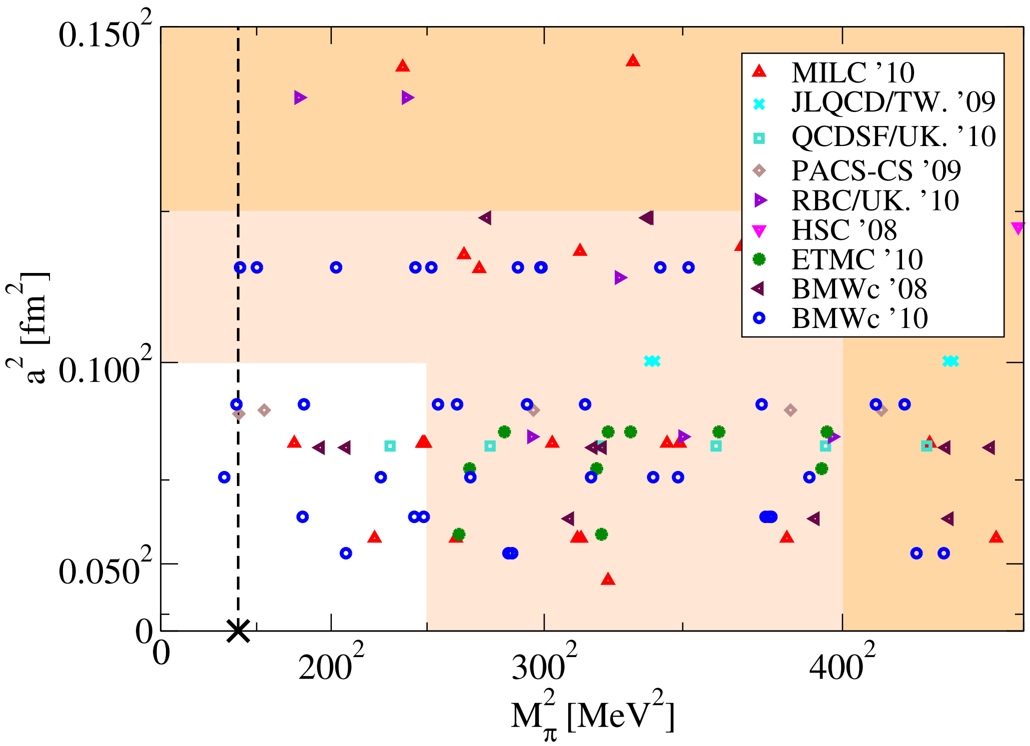
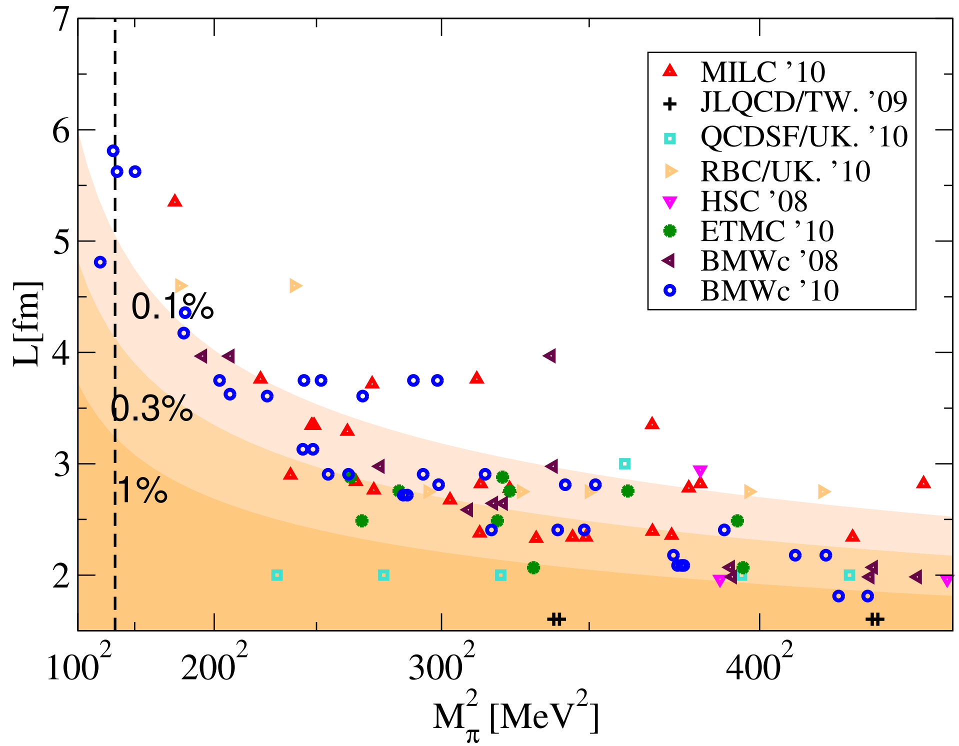




Still only ones there!

☞ begin w/ light quark masses

Light quark masses: motivation

Determine m_u, m_d, m_s *ab initio*

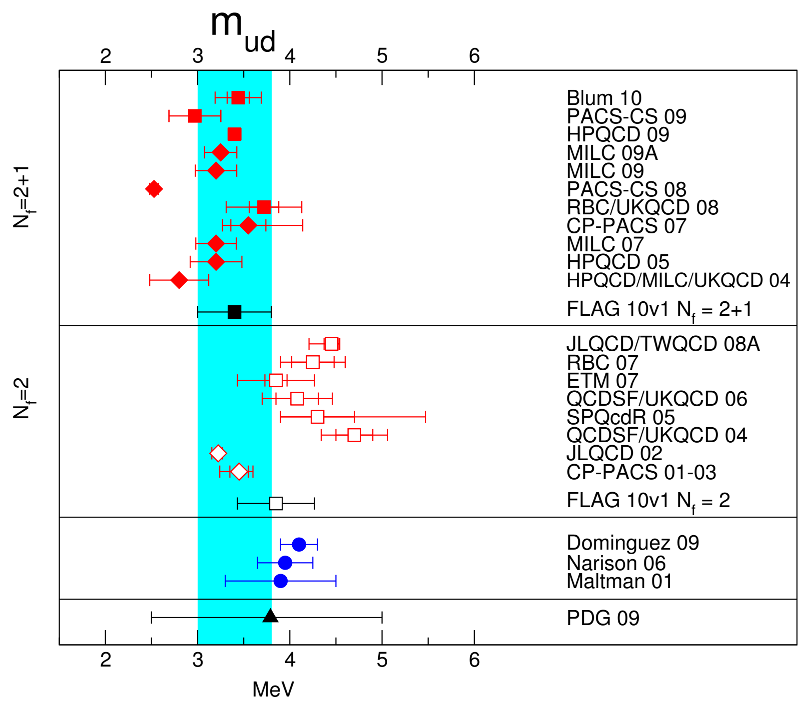
- Fundamental parameters of nature
- Precise values $\rightarrow$ stability of matter, N-N scattering lengths, presence or absence of strong CP violation, etc.
- Information about flavor structure of BSM physics
- Nonperturbative (NP) computation is required
- Would be needle in a haystack problem if not for χSB

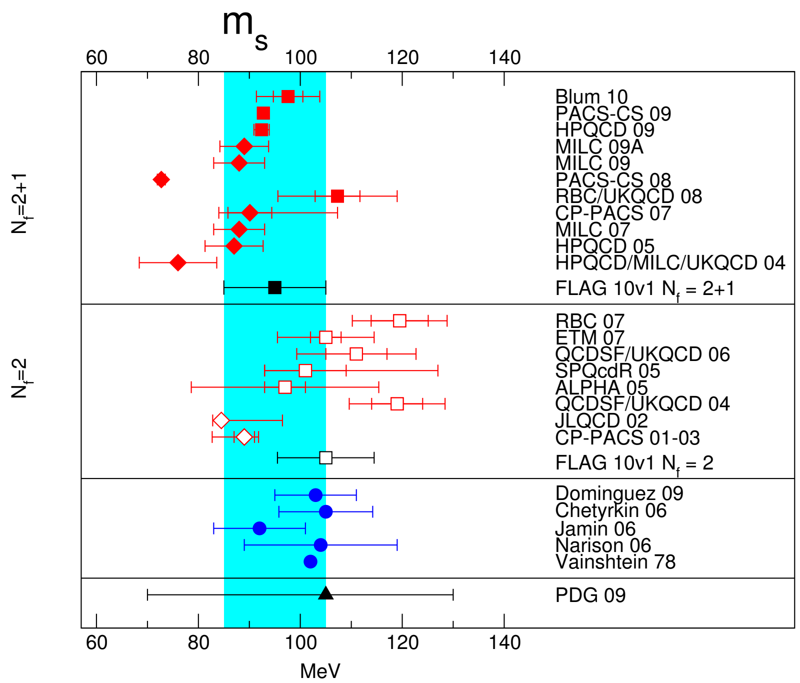
$\Rightarrow$ interesting first "measurement" w/ physical point LQCD

Light quark masses circa Aug. 2010

FLAG $\rightarrow$ analysis of unquenched lattice determinations of light quark masses

(arXiv:1011.4408v1)





$$m_{ud}^{\overline{\rm MS}}(2\,\mathrm{GeV}) = \begin{cases} 3.4(4)\,\mathrm{MeV} & [12\%] \quad \text{FLAG} \\ 2.5 \div 5.0\,\mathrm{MeV} & [30\%] \quad \text{PDG} \end{cases}$$

$$m_{s}^{\overline{\rm MS}}(2\,\mathrm{GeV}) = \begin{cases} 95.(10)\,\mathrm{MeV} & [11\%] \quad \text{FLAG} \\ 70 \div 130\,\mathrm{MeV} & [30\%] \quad \text{PDG} \end{cases}$$

Even extensive study by MILC still has:

- $M_\pi^{\rm RMS} \geq 260\,\mathrm{MeV} \quad \Rightarrow \quad m_{ud}^{\rm MILC,eff} \geq 3.7 \times m_{ud}^{\rm phys}$
- perturbative renormalization (albeit 2 loops)

Quark mass definitions

Standard

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

✓ Only Z_S multiplicative renormalization w/ no pion poles

☞ Use $O(a)$-improved version

Renormalization strategy

Goal

- Convert bare lattice masses to finite renormalized ones ...
- ... fully nonperturbatively ...
- ... with optional accurate conversion to other schemes

Method

- Use RI-MOM scheme nonperturbative renormalization (NPR) (Martinelli et al '95)
  - ... with $S(p) \to \bar{S}(p) = S(p) - \mathrm{Tr}_D[S(p)]/4$ (Becirevic et al '00)
- Compute $Z_S(a\mu, g_0)$ for $\mu \ll 2\pi/a \sim 11 \div 24\,\mathrm{GeV}$

  ✓ $\mu = 1.3\,\mathrm{GeV}$ ✓ $\mu = 2.1\,\mathrm{GeV}$
- Continuum nonperturbative running to high scale $\mu' \gg \Lambda_{QCD}$
- Further conversions in 4-loop PT
- 21 additional $N_f = 3$ RI/MOM simulations at same 5 β's

RI/MOM nonperturbative renormalization

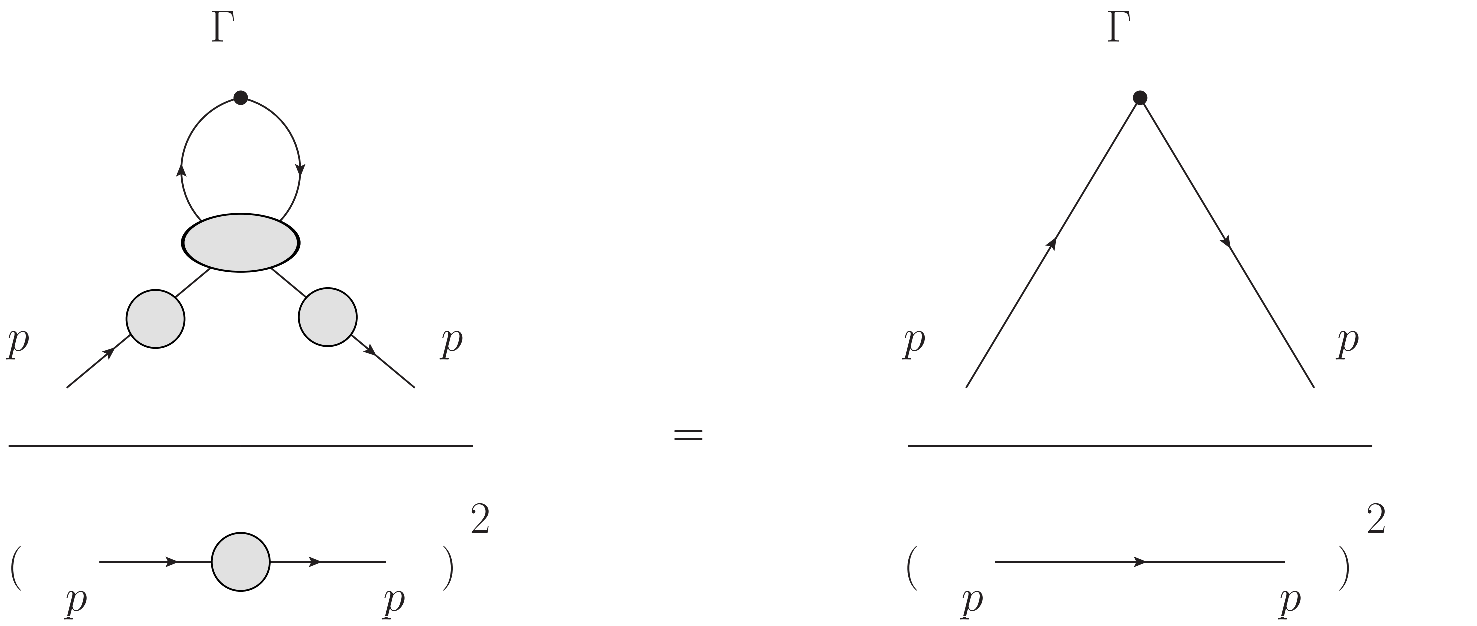
(Martinelli et al '95)

Definition

$$[\bar{q}_1 \Gamma q_2](\mu) = Z_\Gamma^{\mathrm{RI}}(a\mu, g_0)[\bar{q}_1 \Gamma q_2](a)$$

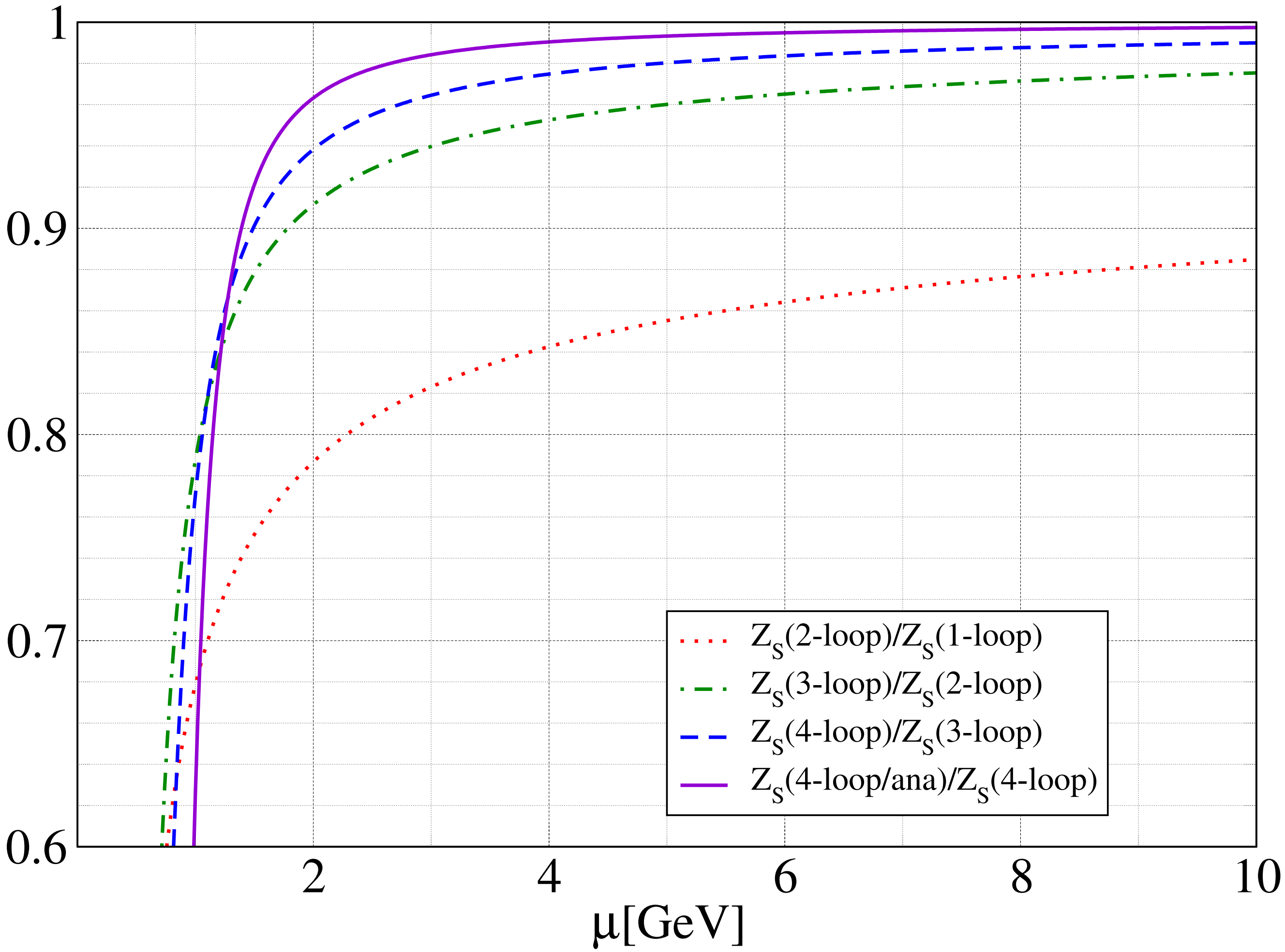
In Landau gauge, compute LHS ratio of quark correlation functions

$$\frac{Z_\Gamma^{\mathrm{RI}}(ap, g_0)}{Z_q^{\mathrm{RI}}(ap, g_0)}$$



Cancel $Z_q^{\mathrm{RI}}(a\mu, g_0)$ by normalizing with LHS of conserved vector current

Optimal RI/MOM scale

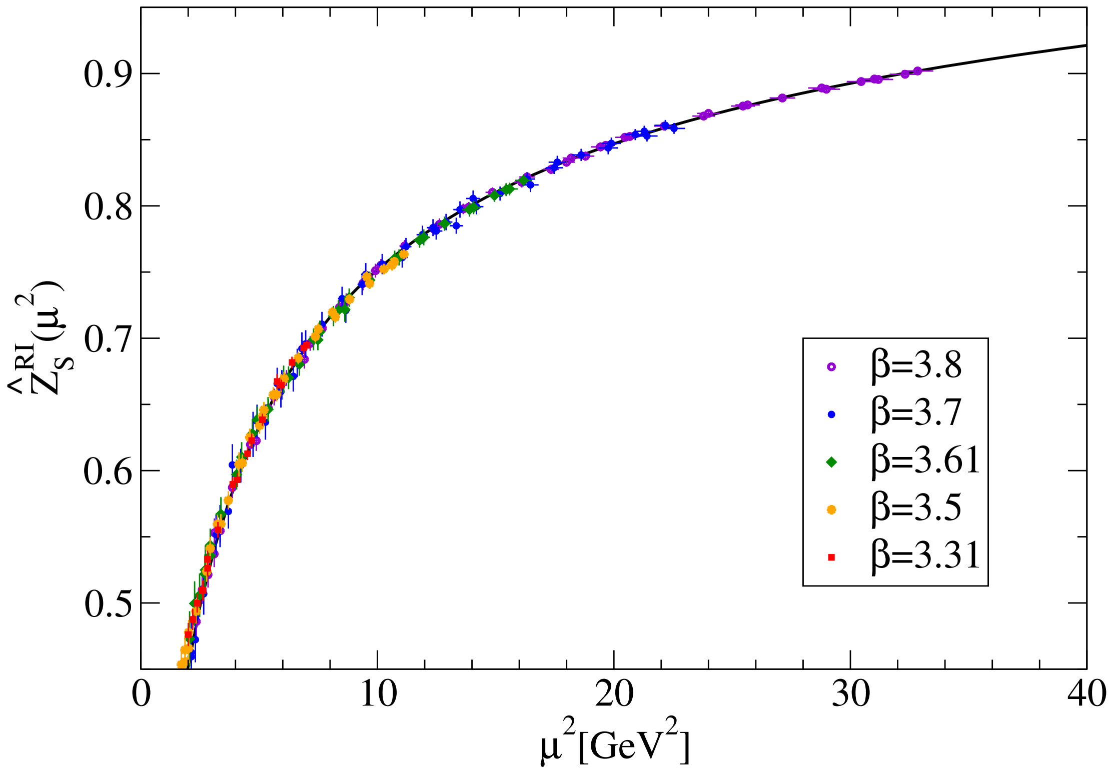


$\Rightarrow \sigma_{\mathrm{PT}} \lesssim 1\%$ for $\mu \gtrsim 4\,\mathrm{GeV}$

Nonperturbative running to 4 GeV

Determine nonperturbative running in continuum limit from (see also Constantinou et al '10, Arthur et al '10)

$$R^{\mathrm{RI}}(\mu, 4\,\mathrm{GeV}) = \lim_{a\to 0} \frac{Z_S^{\mathrm{RI}}(4\,\mathrm{GeV}, a)}{Z_S^{\mathrm{RI}}(\mu, a)}$$



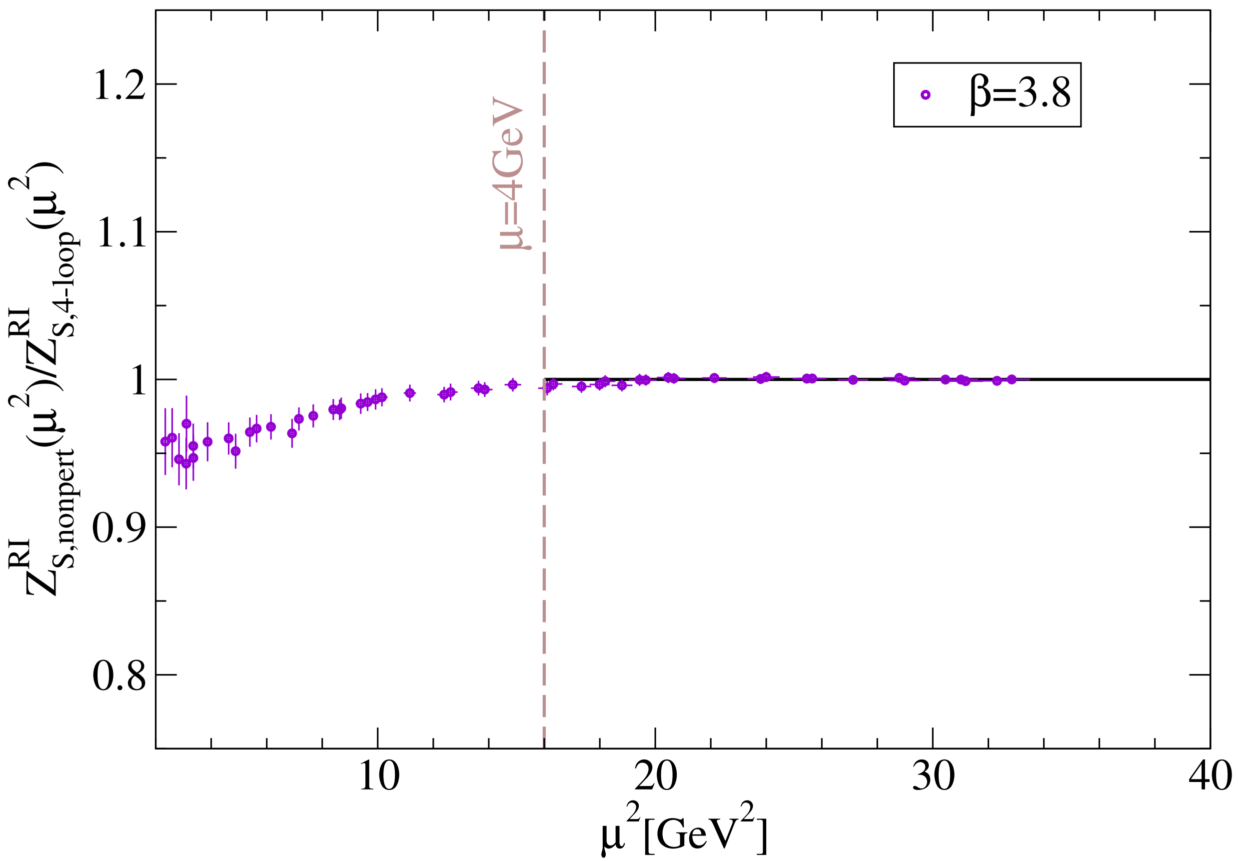
- $3\ \beta$ up to $\mu = 4\,\mathrm{GeV}$
- Running very similar at all $5\ \beta$

$\Rightarrow$ flat and controlled $a \to 0$ extrapolation

Rescaled $Z_S^{\mathrm{RI}}(a\mu, \beta)$ for $\beta < 3.8$ to $\sim$ match $Z_S^{\mathrm{RI}}(a\mu, \beta = 3.8)$

Running beyond 4 GeV

For $\mu > 4\,\mathrm{GeV}$, 4-loop PT and NP running agrees on finest lattice

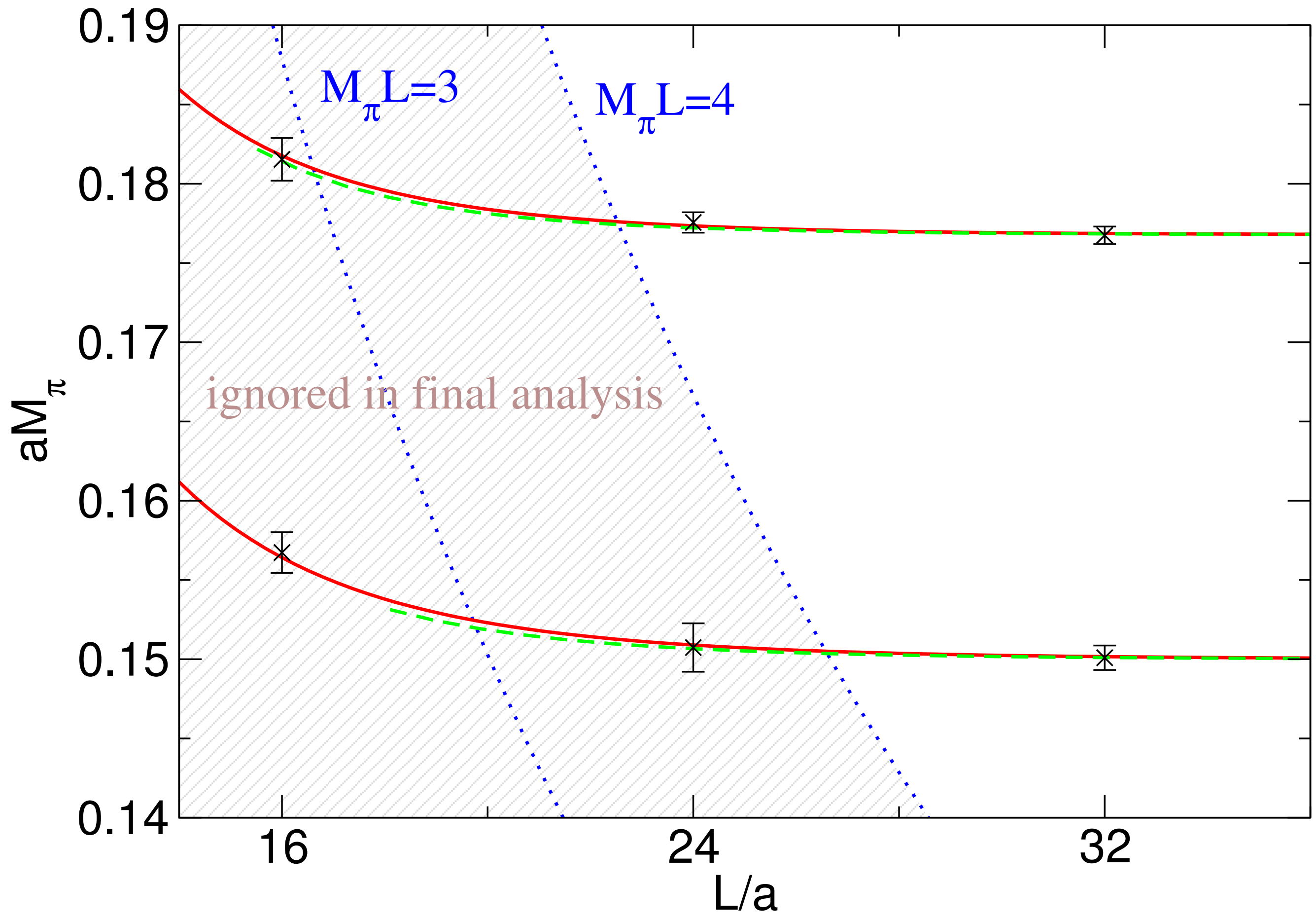


$\Rightarrow$ get RGI masses w/ negligible PT error

$\Rightarrow$ masses in other schemes w/ only errors proper to that scheme

Tiny finite-volume effects

- Dedicated FV runs
- Perfect agreement with FV χPT Colangelo et al '05
- FV effects tiny

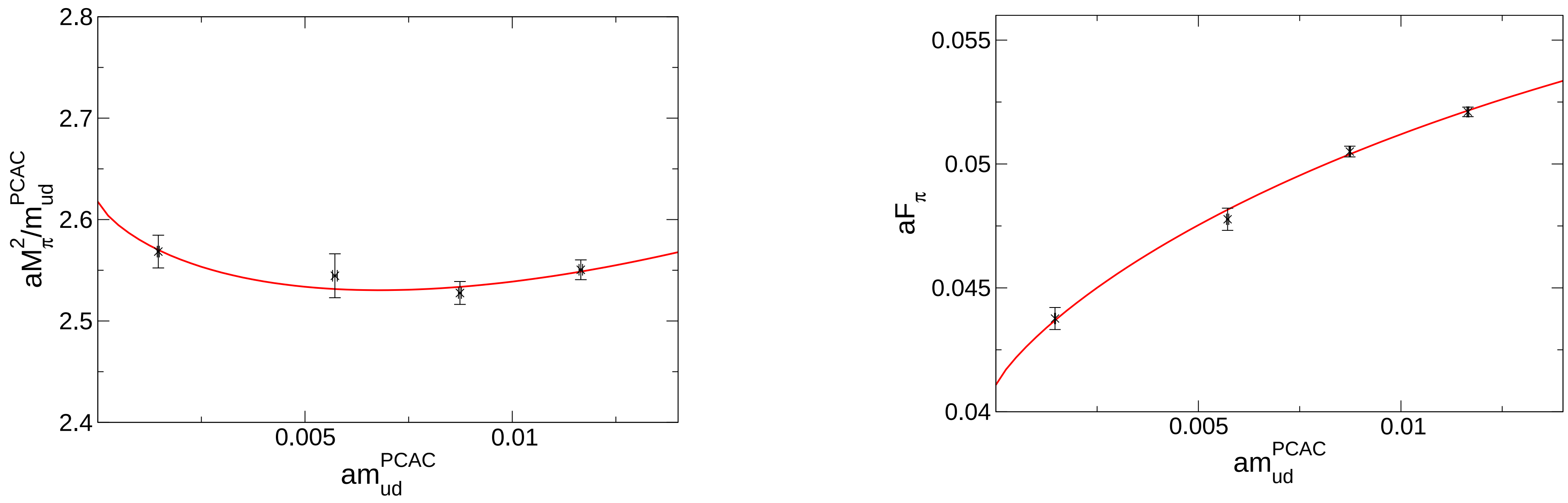


Chiral interpolation to M_π^{ph}

Combined mass interpolation and continuum extrapolation

Illustration of chiral behavior

- Fit to NLO $SU(2)$ χPT (Gasser et al '84)
- Fixed $a \simeq 0.09\,\mathrm{fm}$ and $M_\pi \sim 130 \div 410\,\mathrm{MeV}$



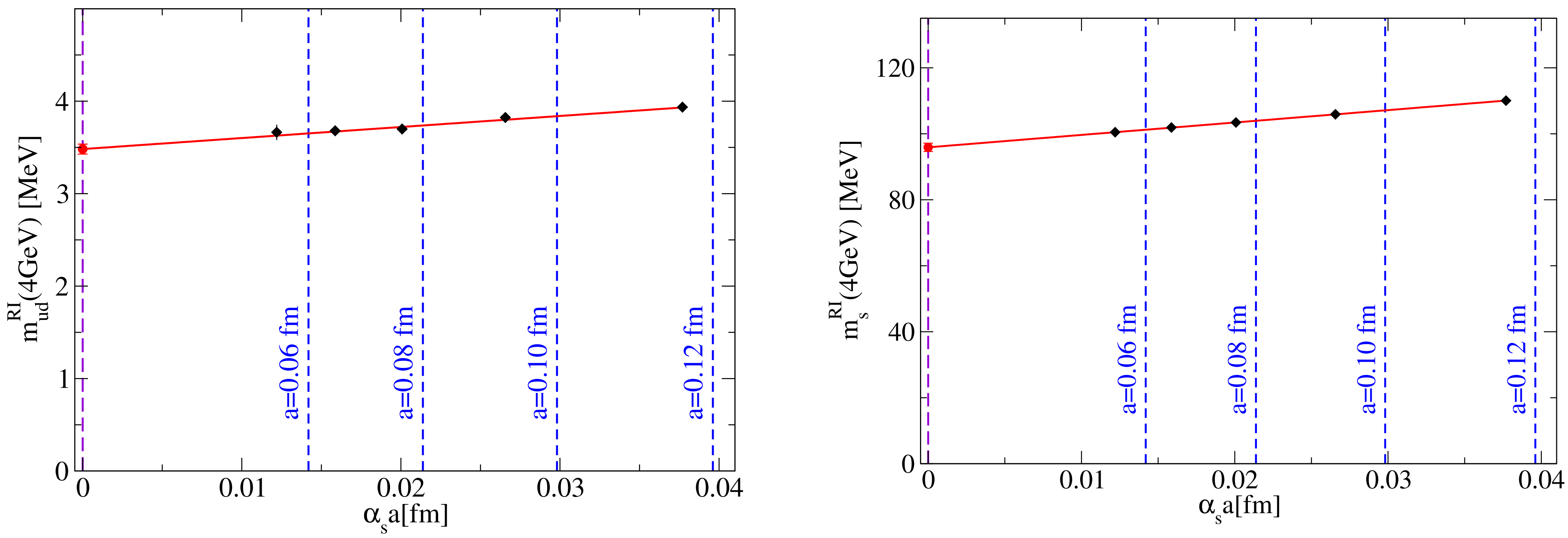
✓ Consistent w/ NLO χPT for $M_\pi \lesssim 410\,\mathrm{MeV}$

$\Rightarrow$ 2 safe interpolation ranges: $M_\pi < 340,\ 380\,\mathrm{MeV}$

$\Rightarrow$ $SU(2)$ NLO χPT & Taylor interpolations to physical point

Continuum extrapolation

- Leading order is $O(\alpha_s a)$
- Allow also domination of sub-leading $O(a^2)$



(Example of continuum extrapolations – errors on points are statistical)

$\Rightarrow$ fully controlled continuum limit

Individual m_u and m_d

Calculation performed in isospin limit:

- $m_u = m_d$
- NO QED

$\Rightarrow$ leave *ab initio* realm

- Use dispersive Q from $\eta \to \pi\pi\pi$

$$Q^2 \equiv \frac{m_s^2 - m_{ud}^2}{m_d^2 - m_u^2}$$

☛ Precise m_{ud} and $m_s/m_{ud} \Rightarrow$

$$m_{u/d} = m_{ud} \left\{ 1 \mp \frac{1}{4Q^2} \left[\left(\frac{m_s}{m_{ud}} \right)^2 - 1 \right] \right\}$$

- Use conservative $Q = 22.3(8)$ (Leutwyler '09)

Systematic error treatment

- 288 full analyses on 2000 boostrap samples
  - 2 correlator time fit ranges
  - 3 NPR procedures
  - 2 continuum forms for NP running
  - 3 chiral forms: $2 \times SU(2)$ χPT, Taylor
  - 2 chiral ranges: $M_\pi < 340, 380\,\mathrm{MeV}$
  - 2 chiral ranges for scale setting channel M_Ω: $M_\pi < 340, 480\,\mathrm{MeV}$
  - 2 continuum forms
- Analyses weighted by fit quality $\Rightarrow$ systematic error distribution
  - Mean $\rightarrow$ final result
  - Std. dev. $\rightarrow$ systematic error
- Statistical error from distribution of means over 2000 samples

Results

	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(4)(3)(10)	2.86(5)(4)(13)	2.15(4)(3)(9)
m_d	4.84(7)(7)(10)	6.39(9)(9)(13)	4.79(7)(7)(9)

$$\frac{m_s}{m_{ud}} = 27.53(20)(8) \qquad \frac{m_u}{m_d} = 0.449(6)(2)(29)$$

Additional consistency checks

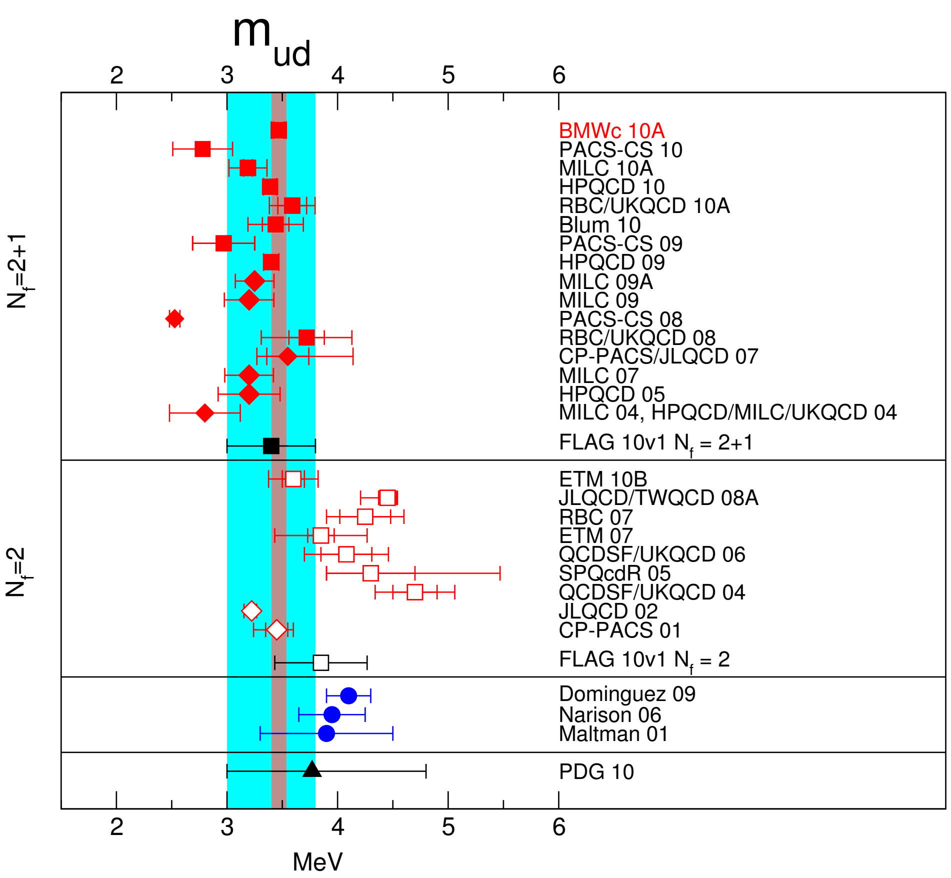
✓ Additional continuum, chiral and FV terms
☞ all compatible with 0

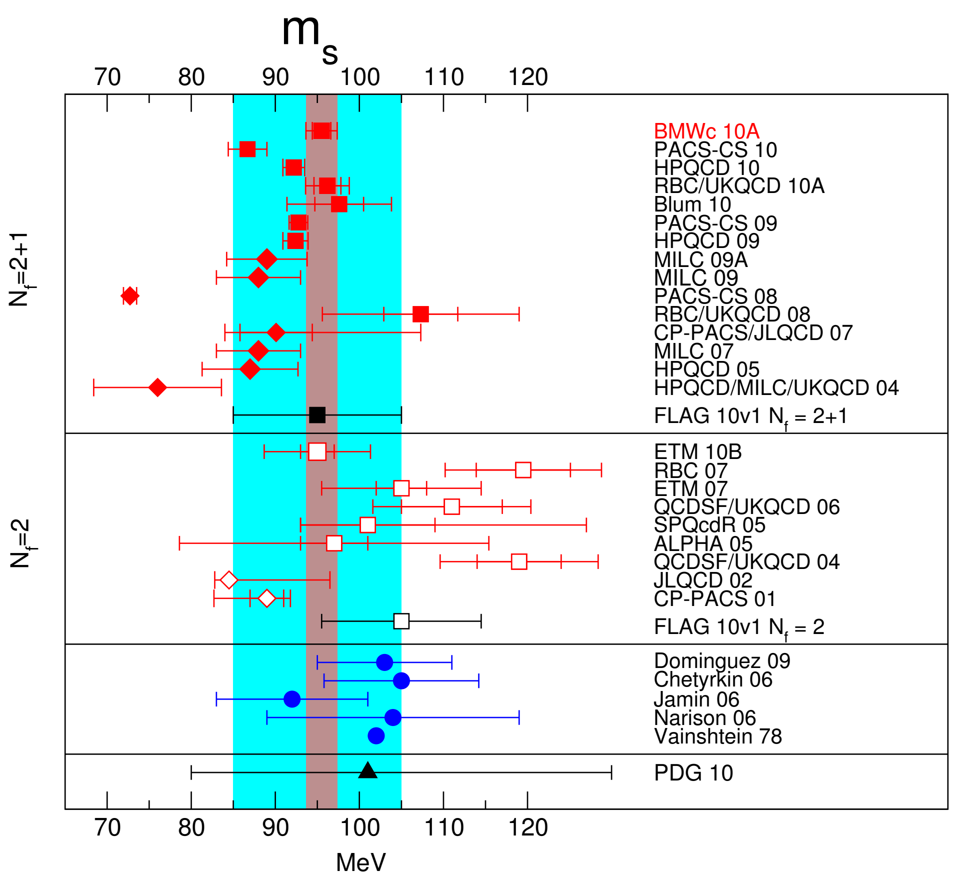
✓ Unweighted final result and systematic error
☞ negligible impact

✓ Use m^{PCAC} only
☞ compatible, slightly larger error

✓ Full quenched check of procedure ☞ cf. reference computation (Garden et al '00)

Comparison





- m_{ud} and m_s are now known to 2%
- … m_u to 5% and m_d to 3% w/ help of phenomenology

Conclusion

- After $>$ 40 years we are finally able to perform fully controlled LQCD computations all the way down to $M_\pi = 135\,\mathrm{MeV}$
- Presented results for light hadron masses and light quark masses
- Have results for F_K/F_π and preliminary results for sigma terms, ρ-width, E+M corrections, ...
- Lattice QCD is undergoing a major shift in paradigm
  - it is now possible to control and reliably quantify all systematic errors with "data" (for 1 or 2 hadron states)

  $\Rightarrow$ we are getting QCD NOT LQCD predictions
  - requires numerous simulations with $M_\pi < 200\,\mathrm{MeV}$ and preferably $\searrow 135\,\mathrm{MeV}$, more than 3 $a < 0.1\,\mathrm{fm}$ and lattice sizes $L \to 4 \div 6\,\mathrm{fm}$
  - requires trying all reasonable analyses of "data" and combining results in sensible way to obtain a reliable systematic error
- Calculations with anything less can yield very interesting results which, however, cannot be considered final