Quark mass determinations from BMW collaboration

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Determination of the Fundamental Parameters in QCD
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SFB
TR55

How to compute quark masses?

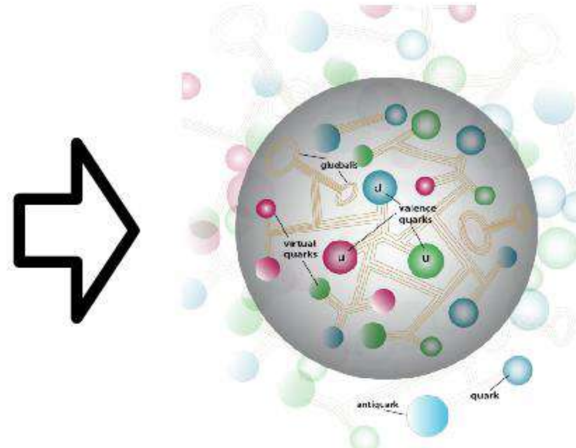
Problem:

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

☞Basic recipie:

- Solve QCD for various quark masses

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\Psi}(\mathrm{i} D_\mu \gamma^\mu - m)\Psi$$

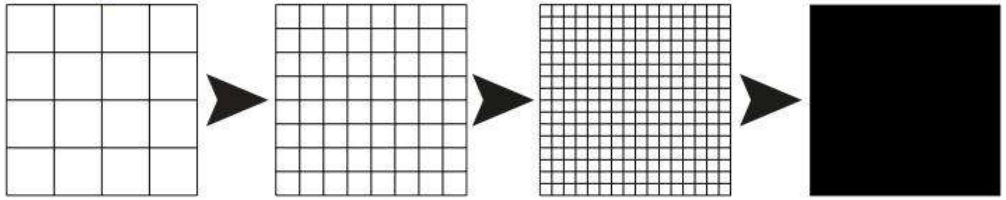


- Compare some results (e.g. m_π, m_K, m_Ξ/m_Ω) with experiment
- Find quark masses that give correct physical results
- Renormalize

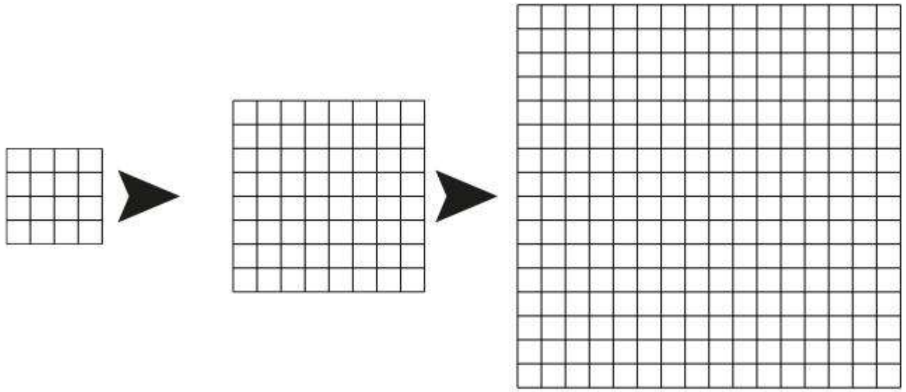
Lattice

Lattice QCD=QCD when

- Cutoff removed (continuum limit)



- Infinite volume limit taken

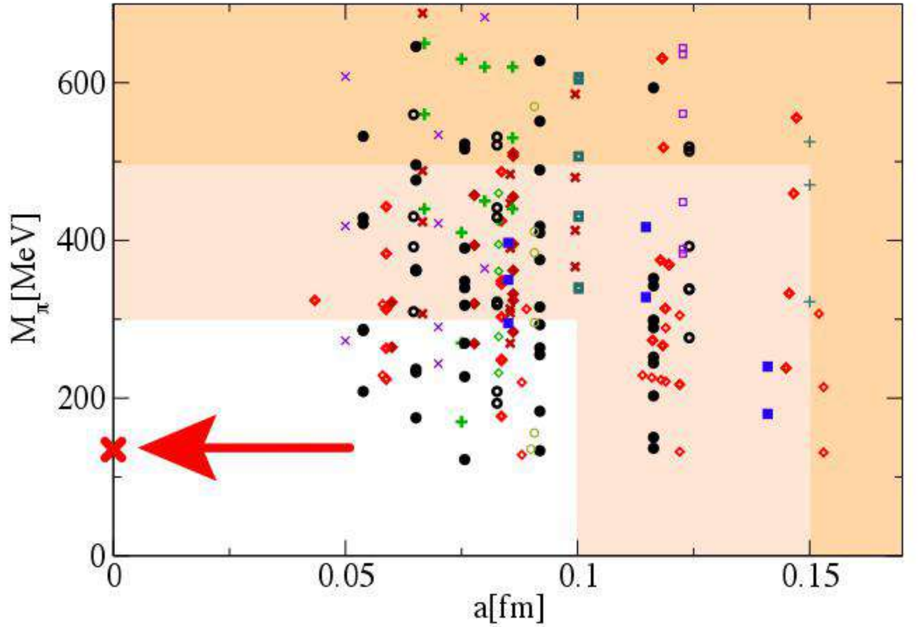


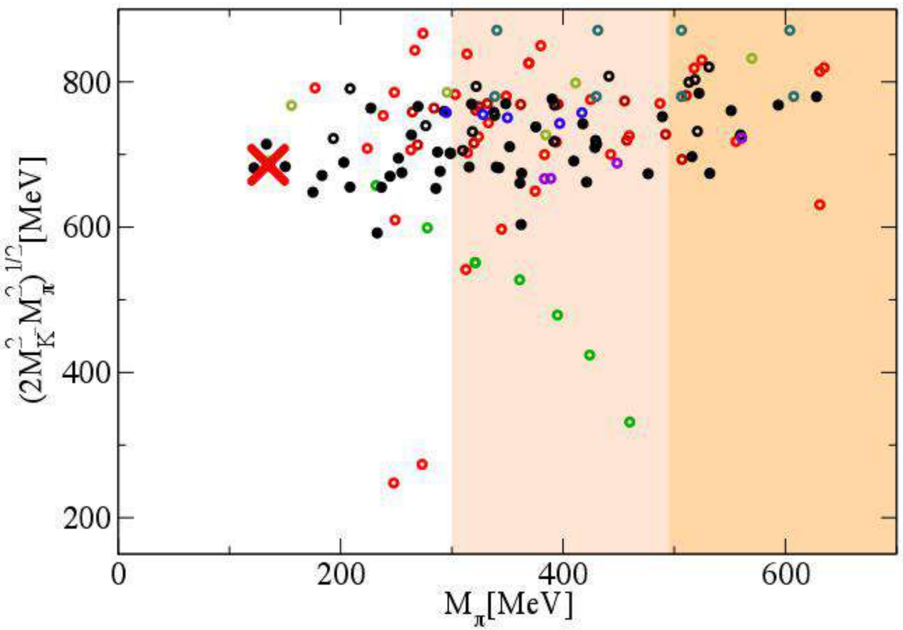
- At physical hadron masses (Especially π)
  - Numerically challenging to reach light quark masses

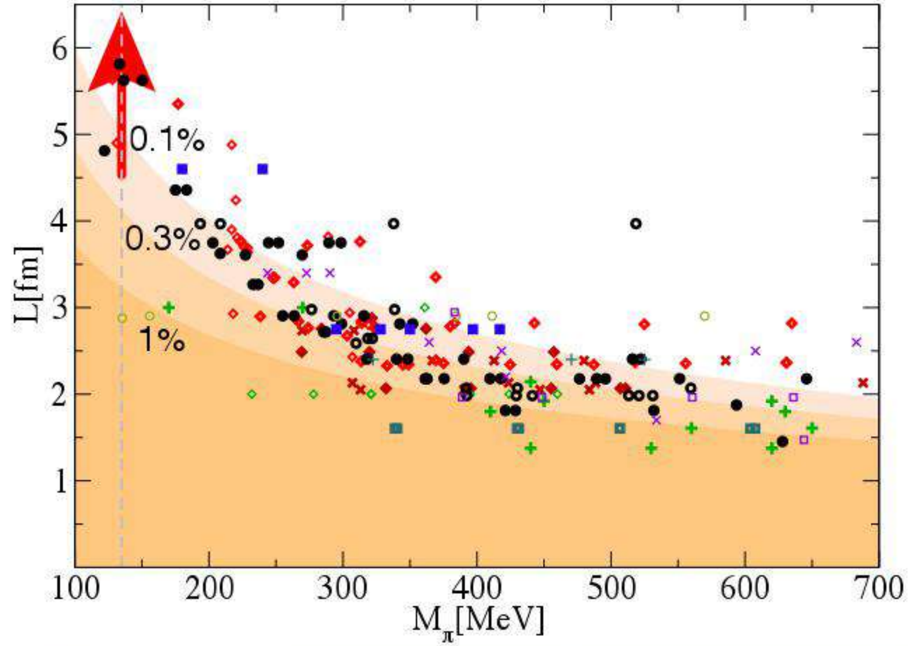
Statistical error from stochastic estimate of the path integral

Extracting a physical prediction

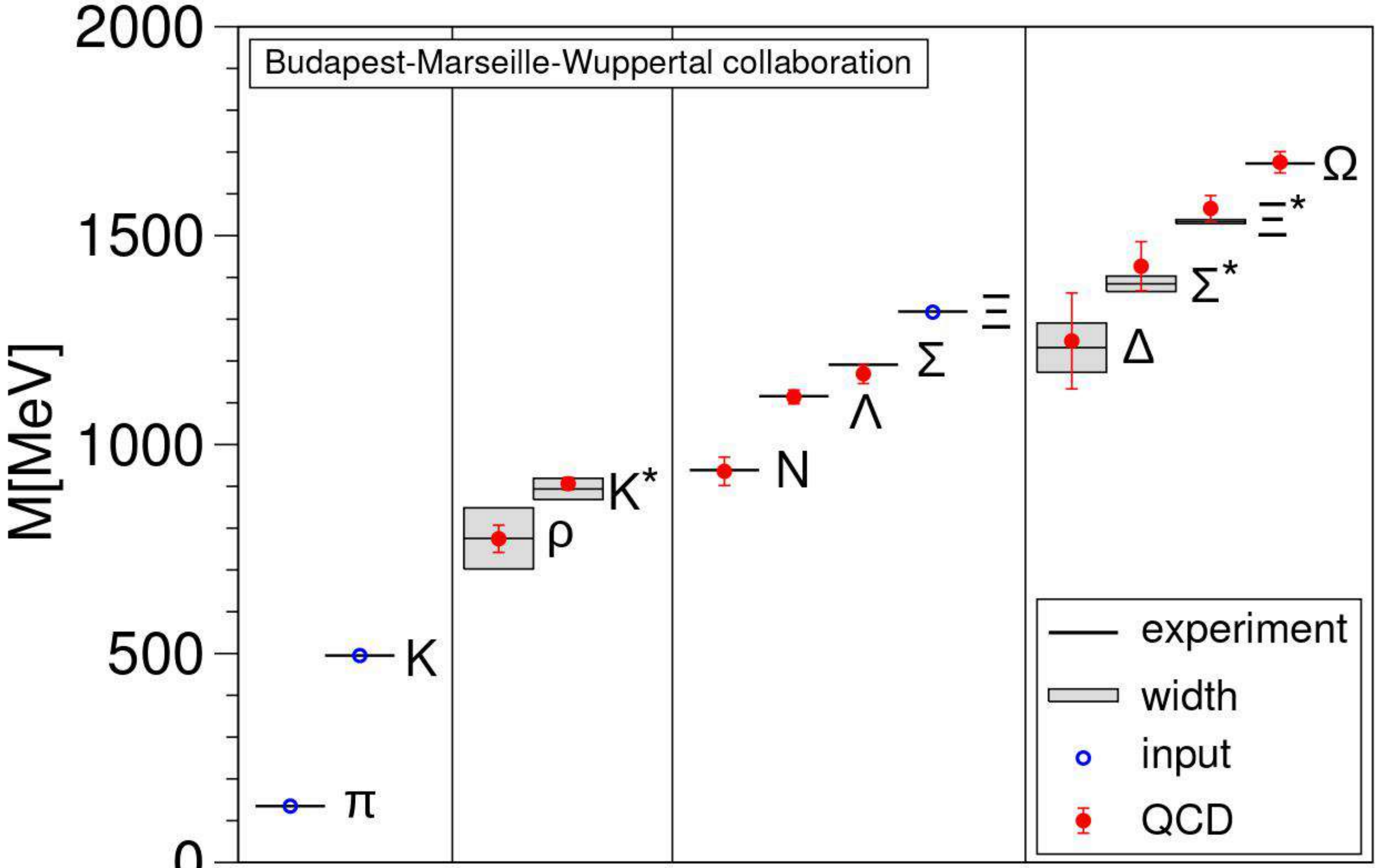
- Compute target observable
- Identify physical point
- Extrapolate to physical point







Physical point from hadron spectrum



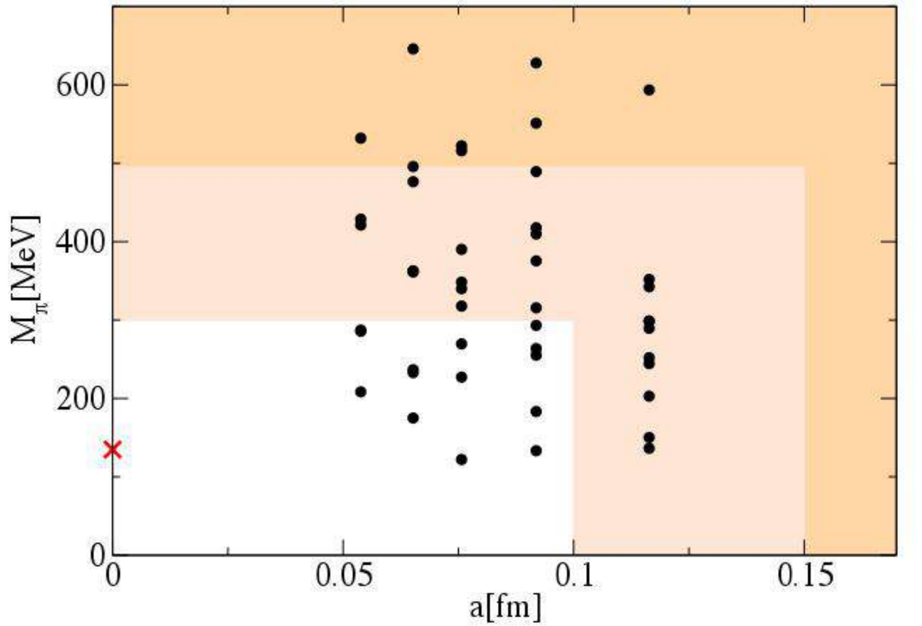
(BMWc, 2008)

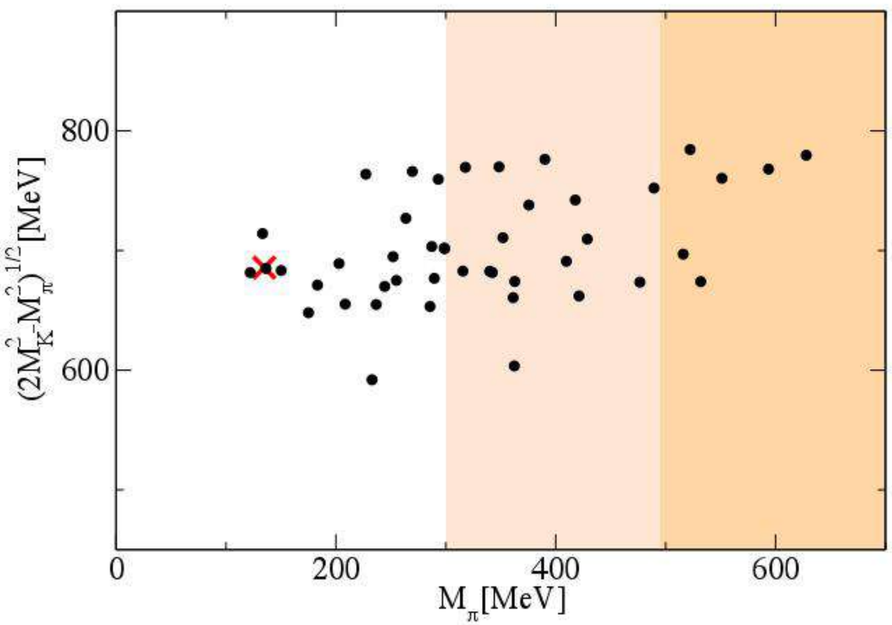
In this talk:

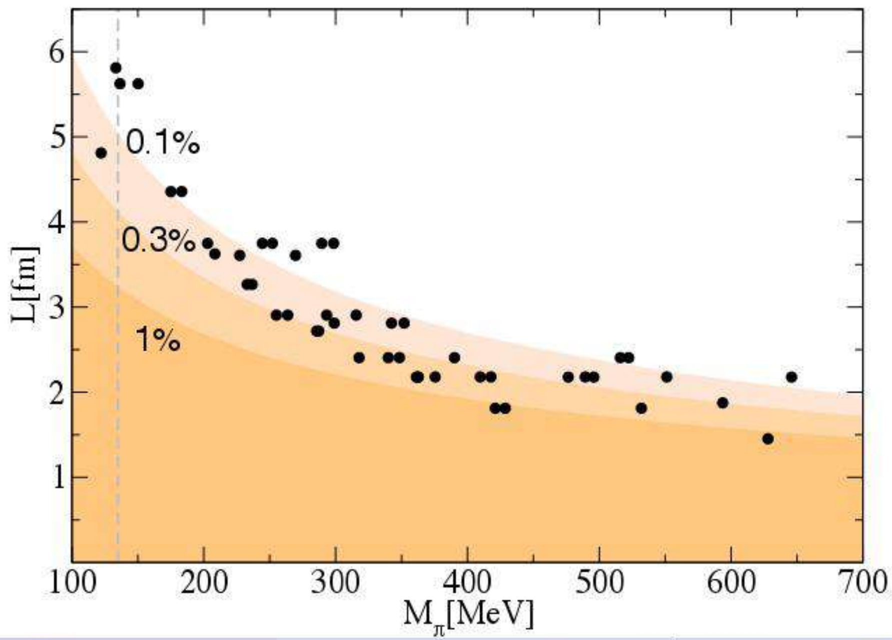
- Computing m_{ud}, m_s in QCD, Wilson type quarks
  - Action and ensembles
  - RI-MOM renormalization, nonperturbative running
  - Ratio-difference method of quark mass extraction
  - Physical point extrapolation and systematic errors
- Splitting $\delta m = m_u - m_d$ in QCD+QED, Wilson type quarks
  - QED on the lattice
  - Finite volume effects
  - Physical point extrapolation and systematic errors
- Precision determination of m_s/m_{ud} in QCD, staggered quarks
  - Motivation for staggered
  - Action and ensembles
  - Extraction techniques
  - Physical point extrapolation and systematic errors

Our ensembles

- Wilson type 2-HEX clover
- Tree level Lüscher-Weisz
- Simple: no parameter tuning
- Small chiral symmetry breaking

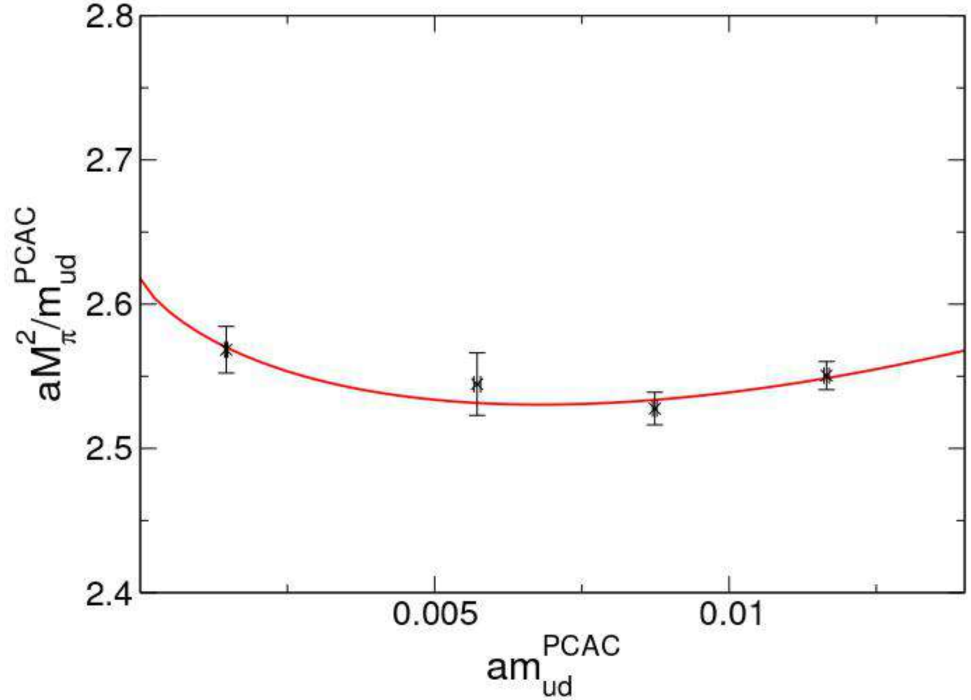


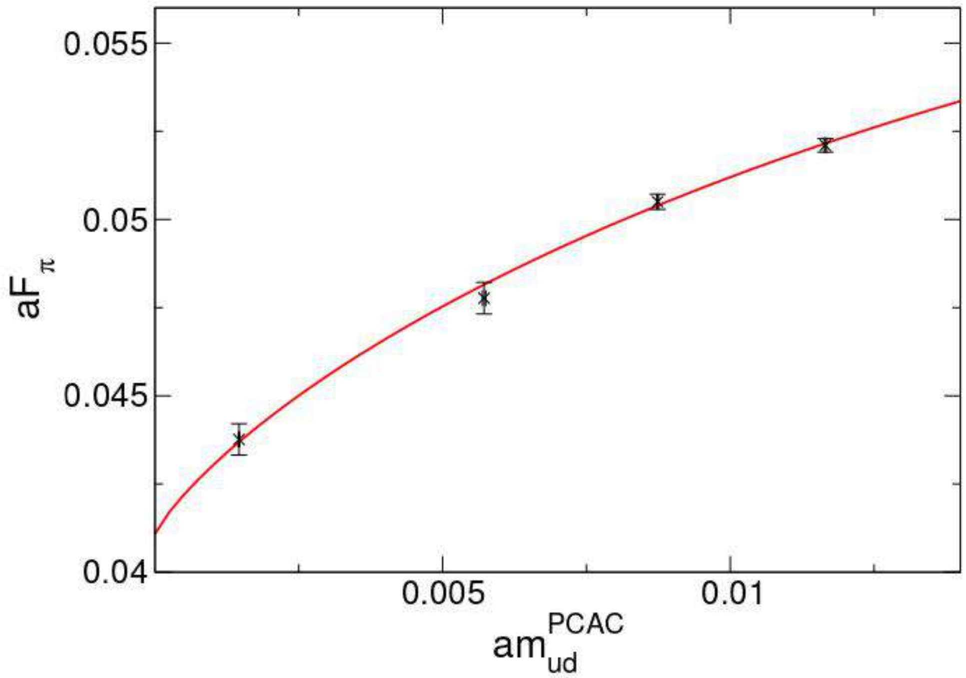




Chiral interpolation

- 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

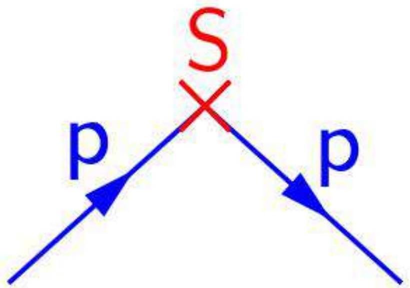
➤ We use $SU(2)$ χPT and Taylor interpolation forms

Renormalization

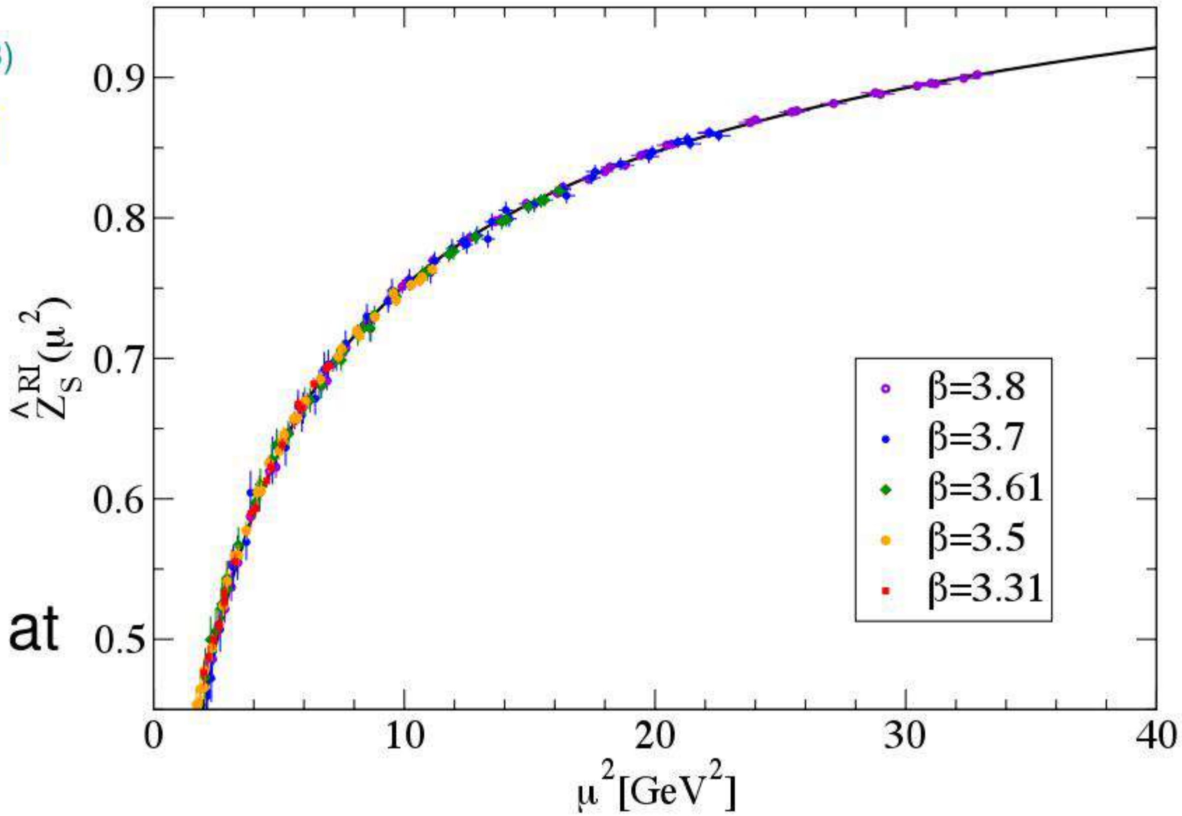
- Quark masses logarithmically divergent ($a \to 0$) ➛ renormalization
- Usual scheme $\overline{\text{MS}}$: perturbatively defined

☞ RI-MOM scheme (Martinelli et. al. 1993)

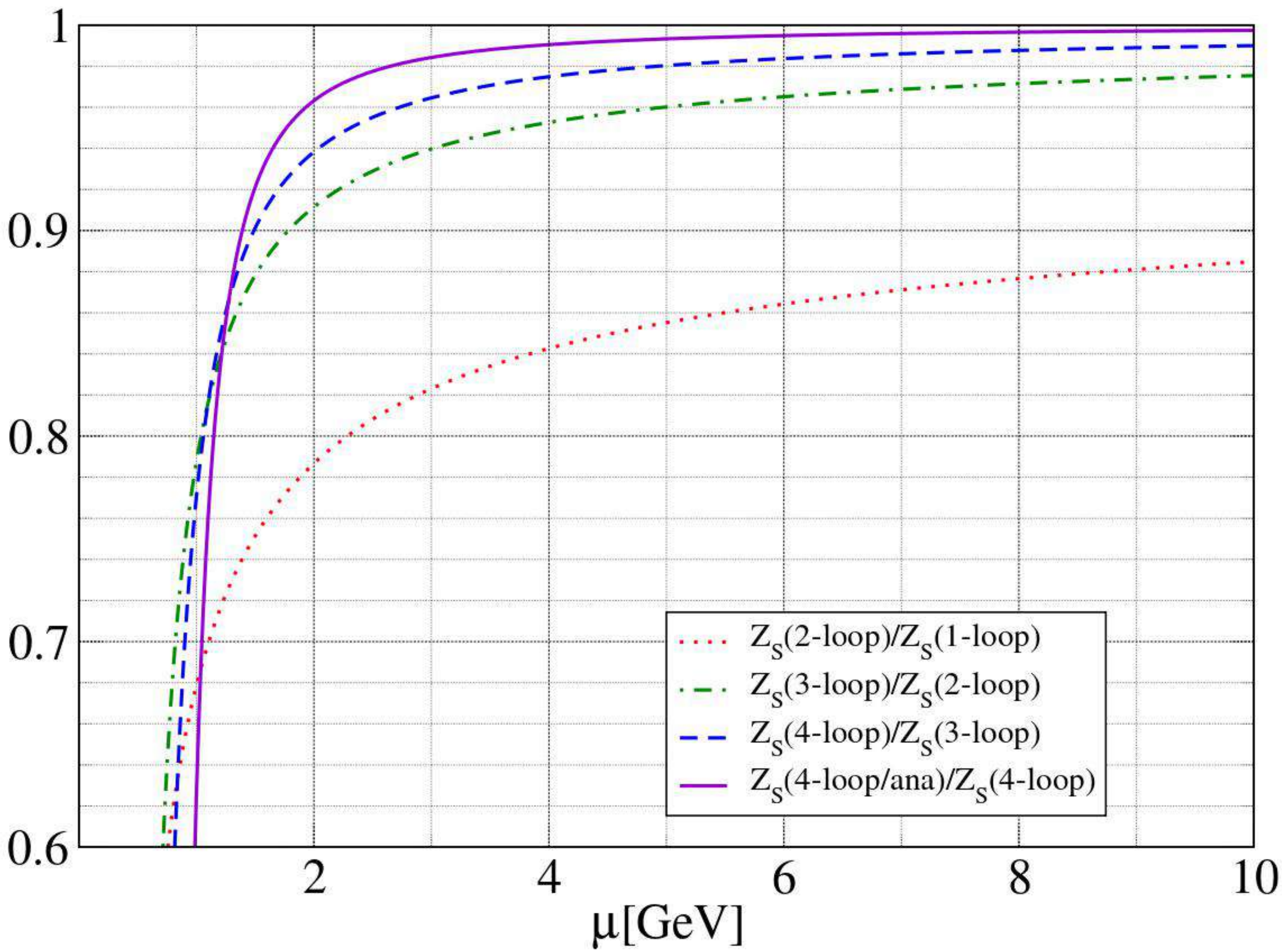
- Matrix elements of off-shell quarks in fixed gauge



- Renormalization condition: at $p^2 = \mu^2$ matrix element assumes tree level value

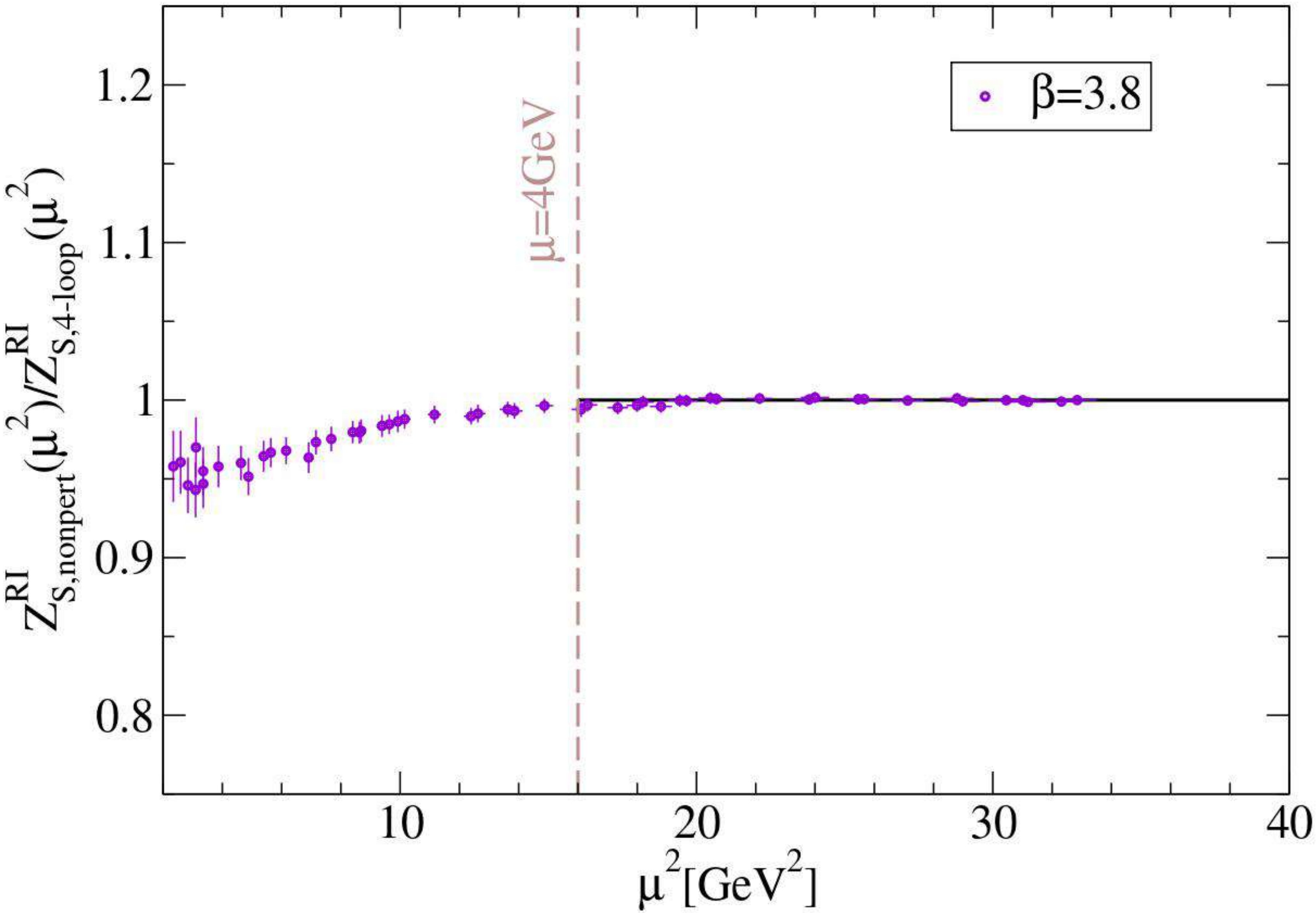


Desired scale in RI-MOM scheme



(Chetyrkin, Retey, 1999)

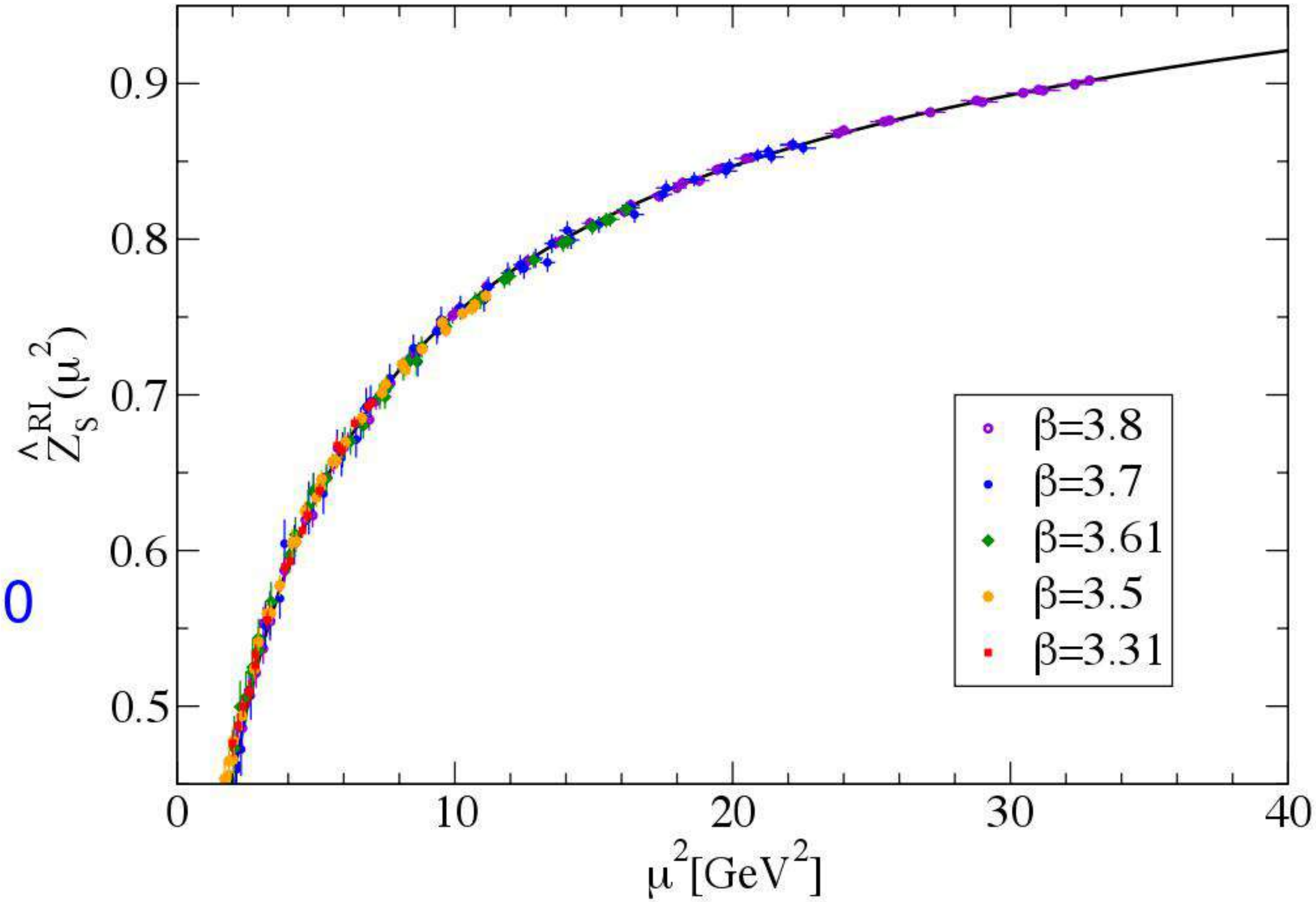
Renormalization: contact with perturbation theory



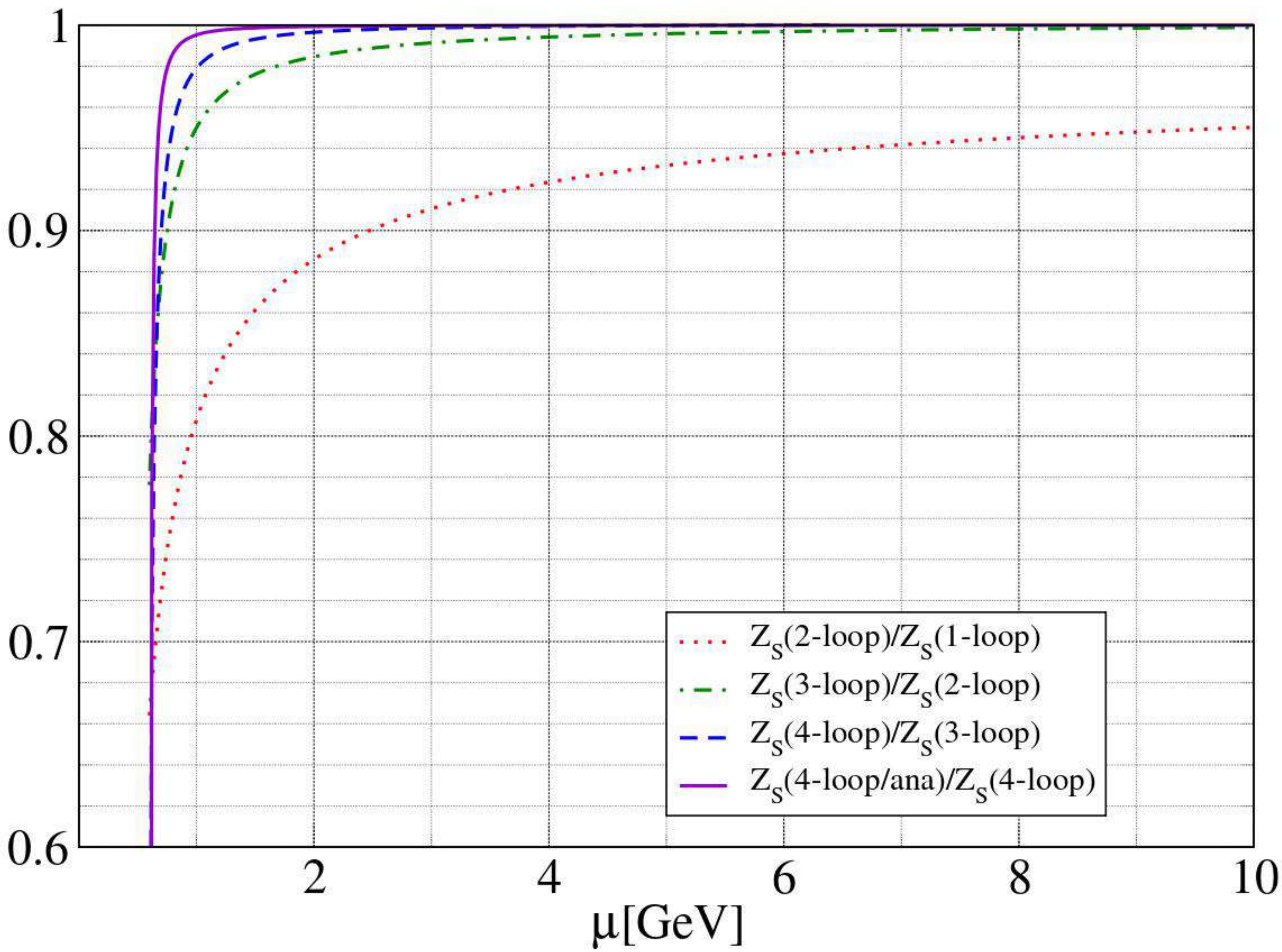
Nonperturbative running

- Contact with PT only for finest lattice spacings
- Match different β onto each other for low μ, finite m_r

- Match at finite m_r
- Extract Z_s ratios and iterate matching
- Extrapolate $m_r \to 0$ at high μ



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



(Cetyrkin 1997; Vermaseren, Larin, van Ritbergen, 1997)

Quark mass definitions

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

Better use

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

- $d = m^{\text{bare}}_s - m^{\text{bare}}_{ud}$
- $d^{\text{ren}} = \frac{1}{Z_S} d$

- $r = m^{\text{PCAC}}_s / m^{\text{PCAC}}_{ud}$
- $r^{\text{ren}} = r$

and reconstruct

- $m^{\text{ren}}_s = \frac{1}{Z_S} \frac{rd}{r-1}$
- $m^{\text{ren}}_{ud} = \frac{1}{Z_S} \frac{d}{r-1}$

✓ 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)

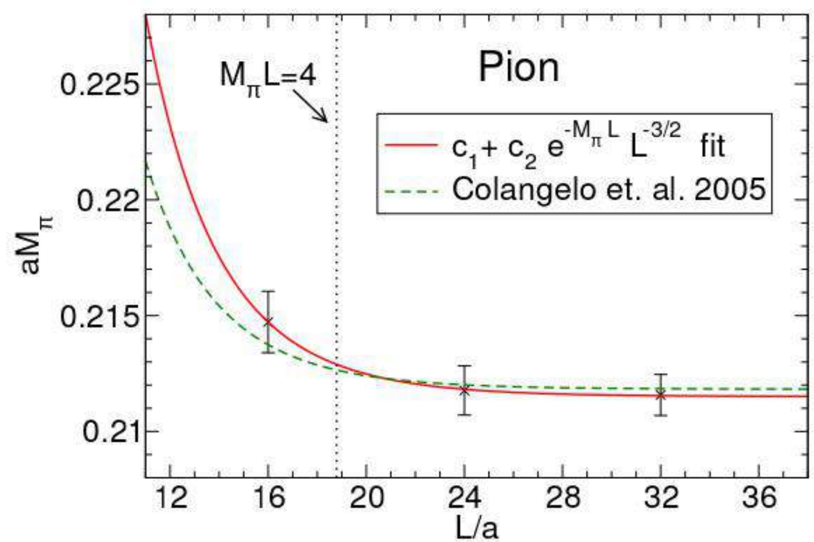
Finite volume effects from virtual pions

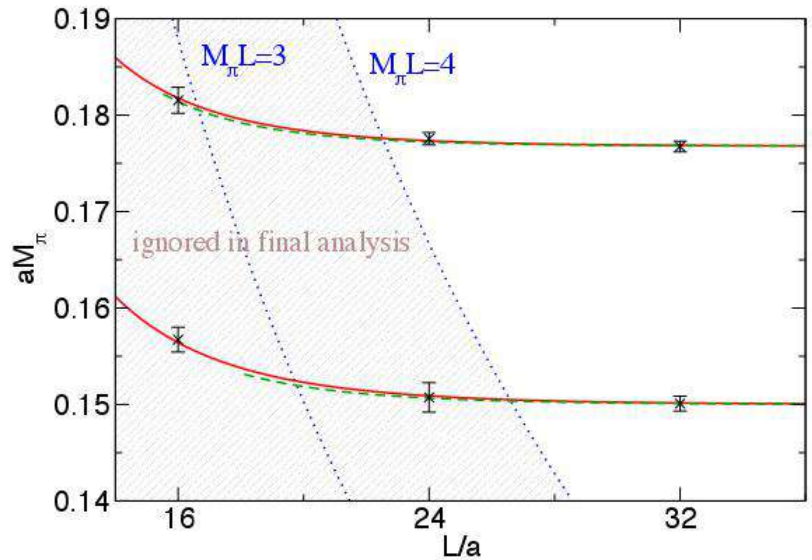
Goal:

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

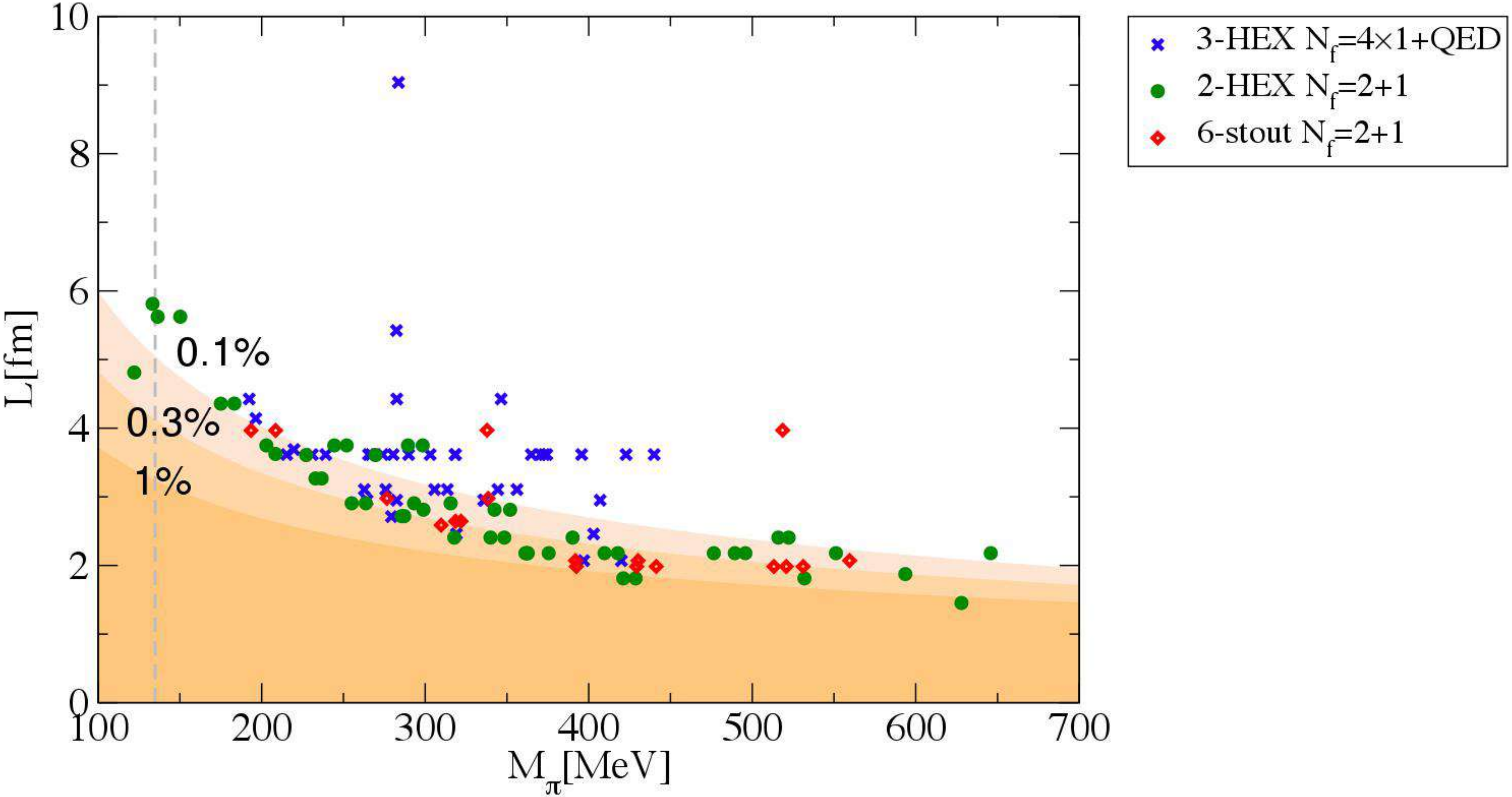
Method:

- 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)

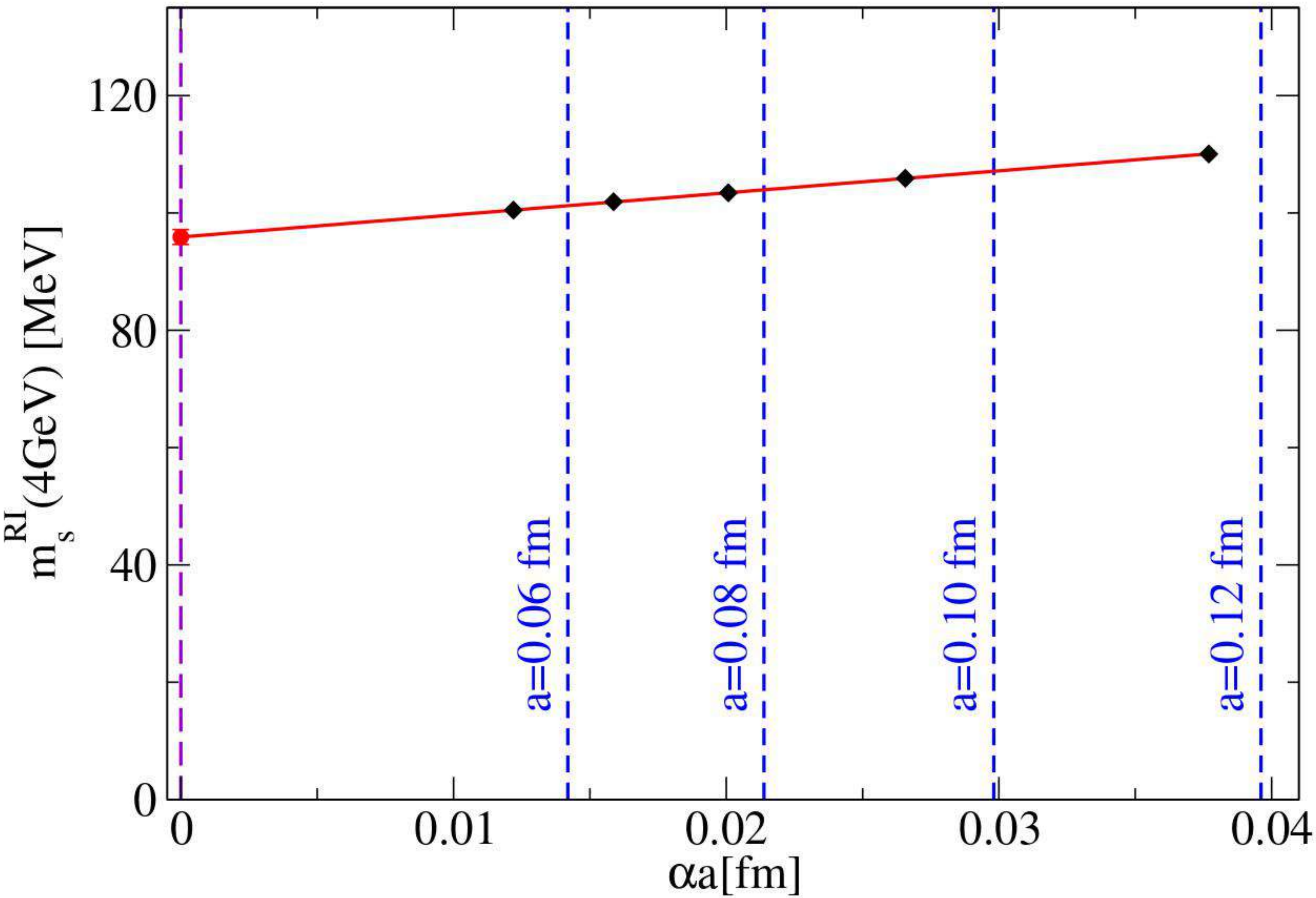




Landscape L vs. M_π



Continuum limit



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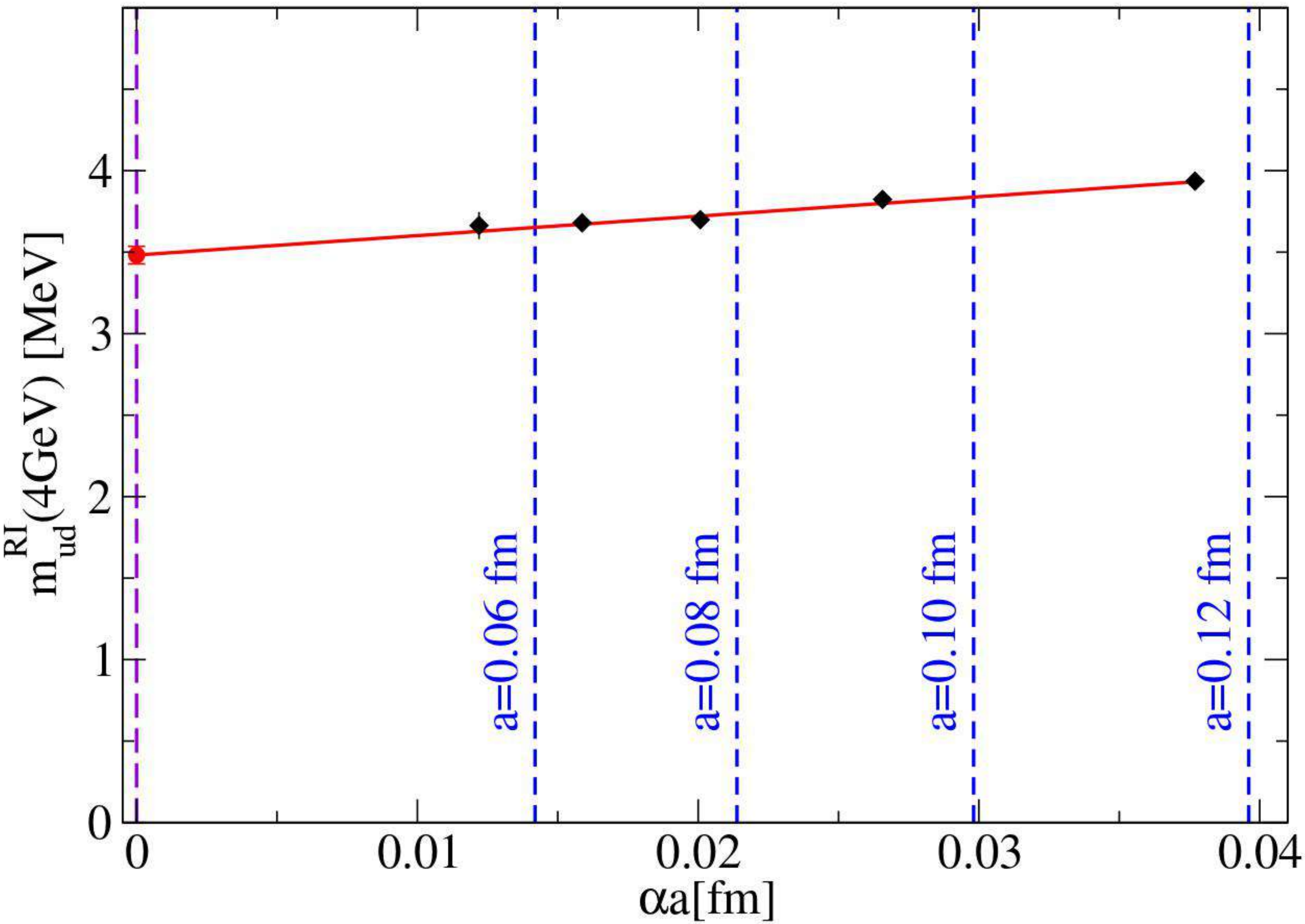

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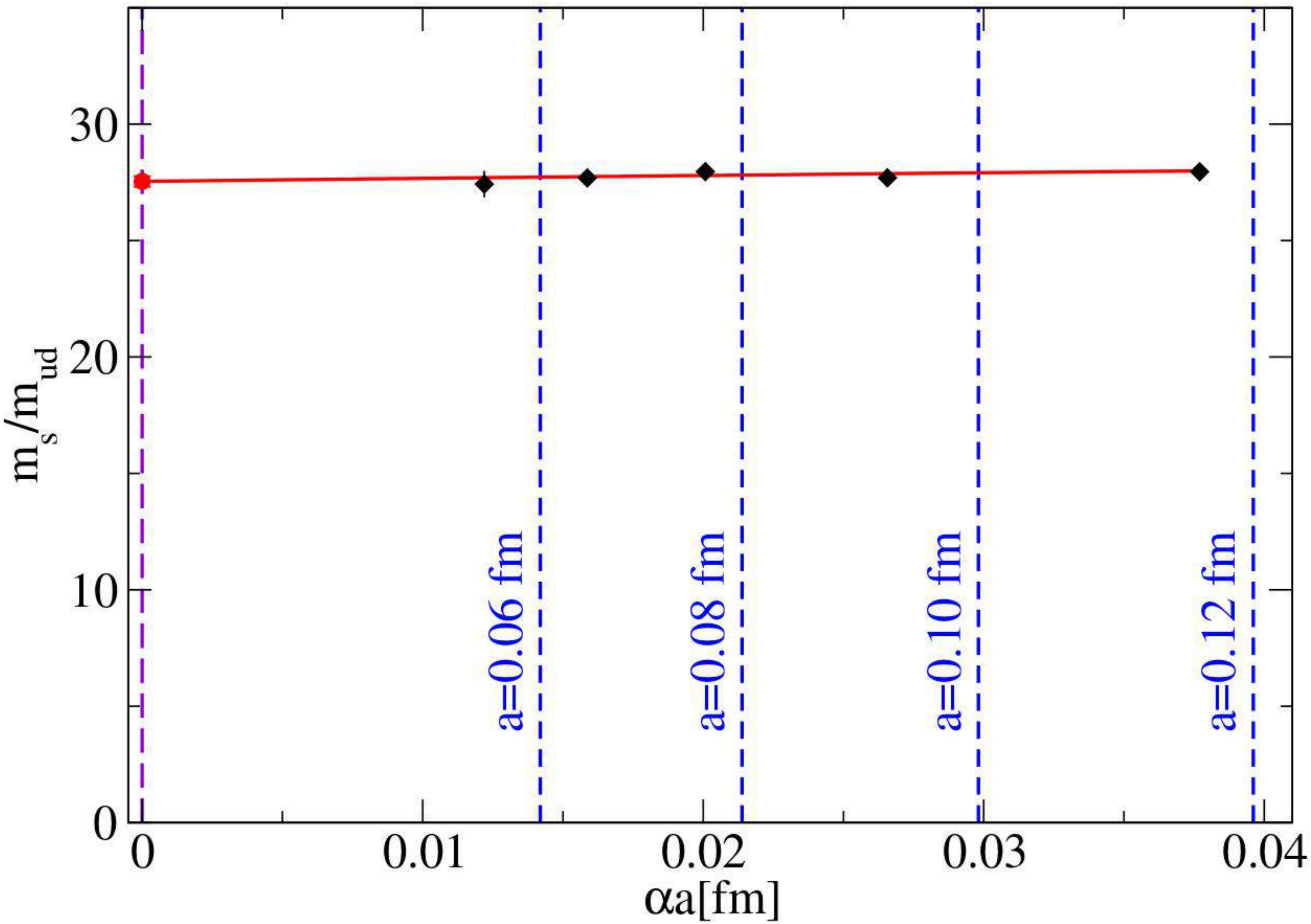
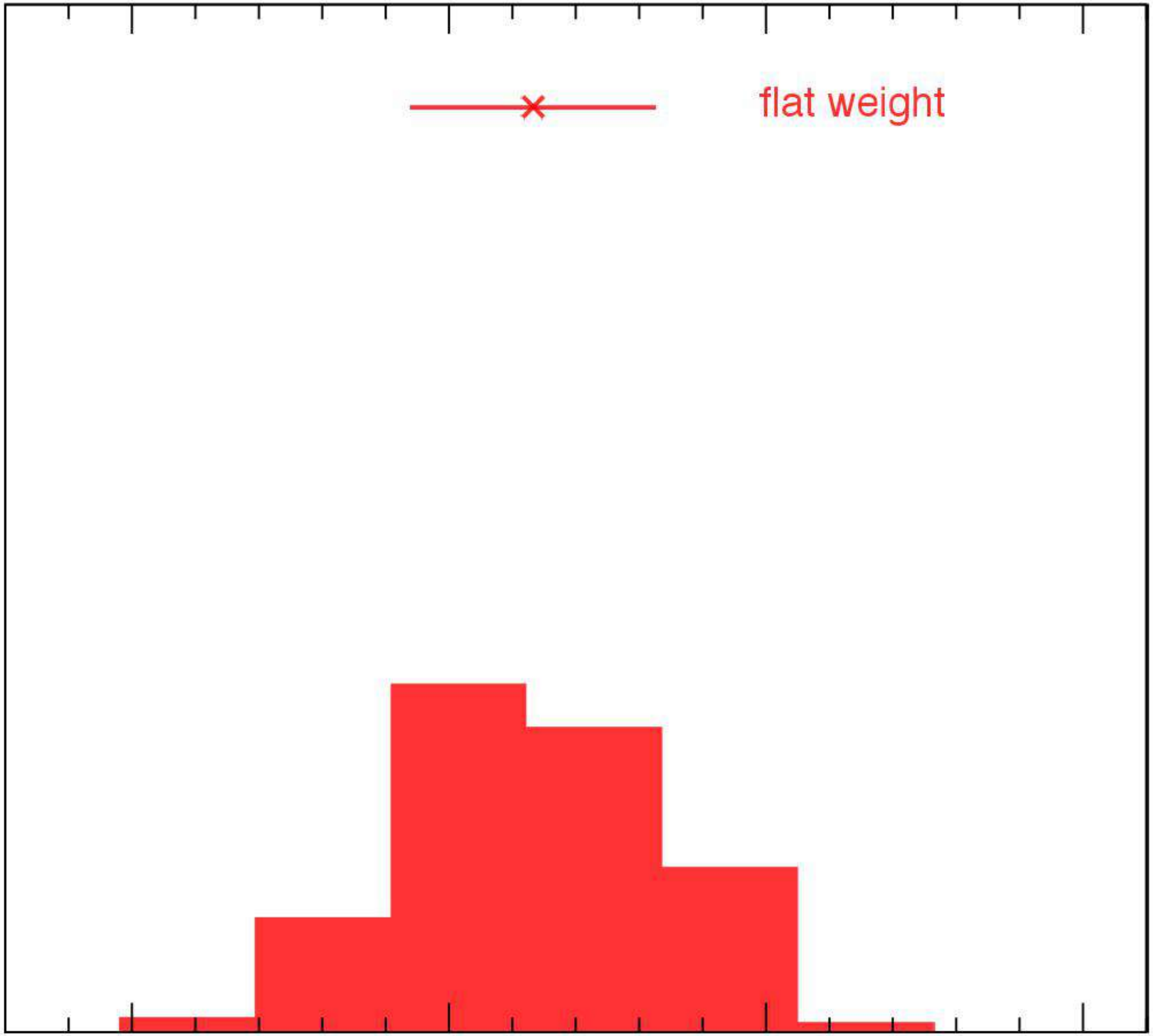


Systematic error treatment

One conservative strategy for systematics:

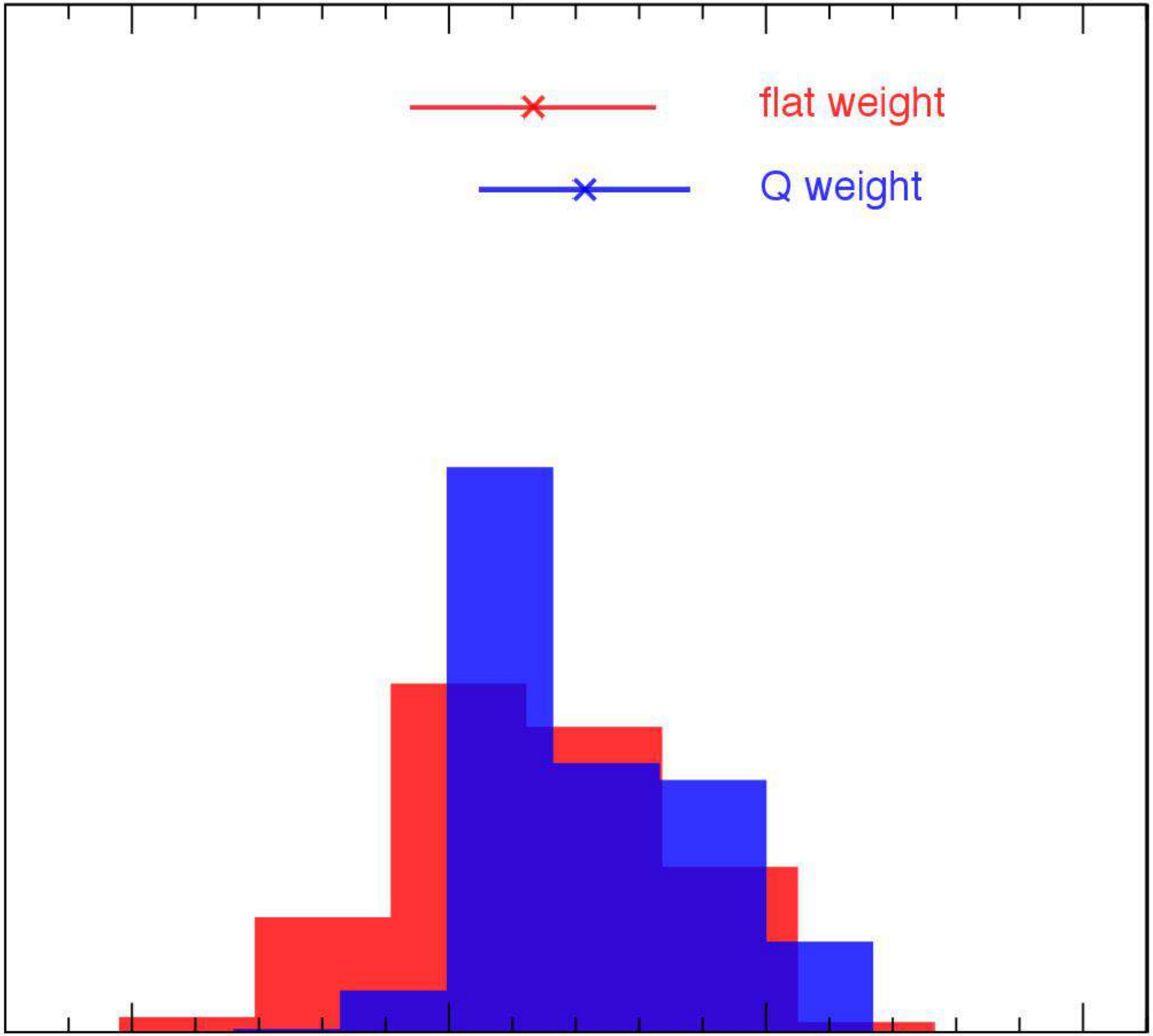
- Identify all higher order effects you have to neglect
- For each of them:
  - Repeat the entire analysis treating this one effect differently
  - Add the spread of results to systematics
- Important:
  - Do not do suboptimal analyses
  - Do not double-count analyses
- Error sources considered:
  - Plateaux range (Excited states)
  - M_π, M_K interpolations
  - Renormalization: NP running mass and matching scale
  - Higher order FV effects
  - Continuum extrapolation

Systematic error



- Perform O(10000) analyses
- Difference: higher order effects
- Draw histogram of results
- Different weights possible
- Crosscheck agreement

Systematic error



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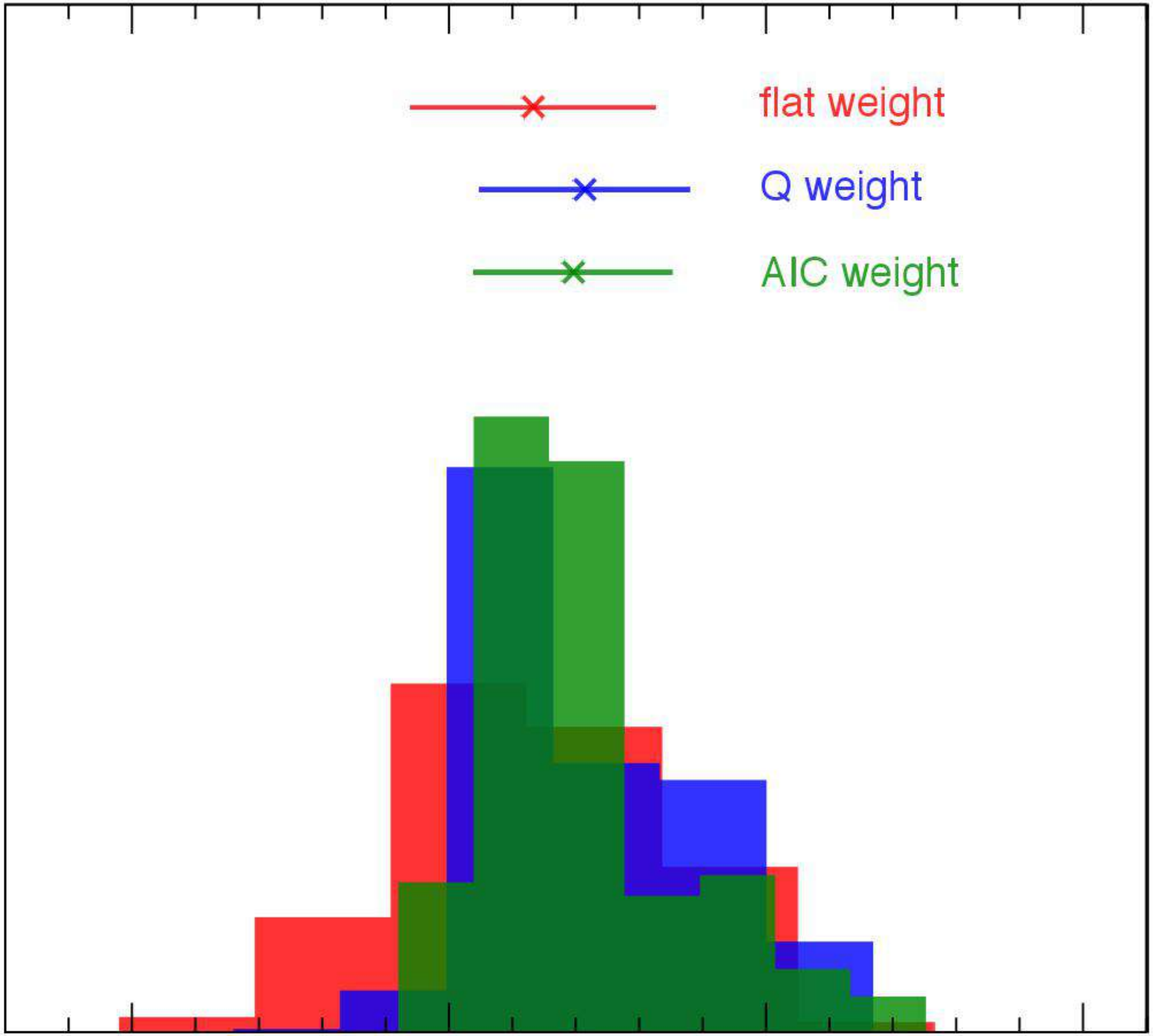


- Perform O(10000) analyses
- Difference: higher order effects
- Draw histogram of results
- Different weights possible
- Crosscheck agreement

Final result

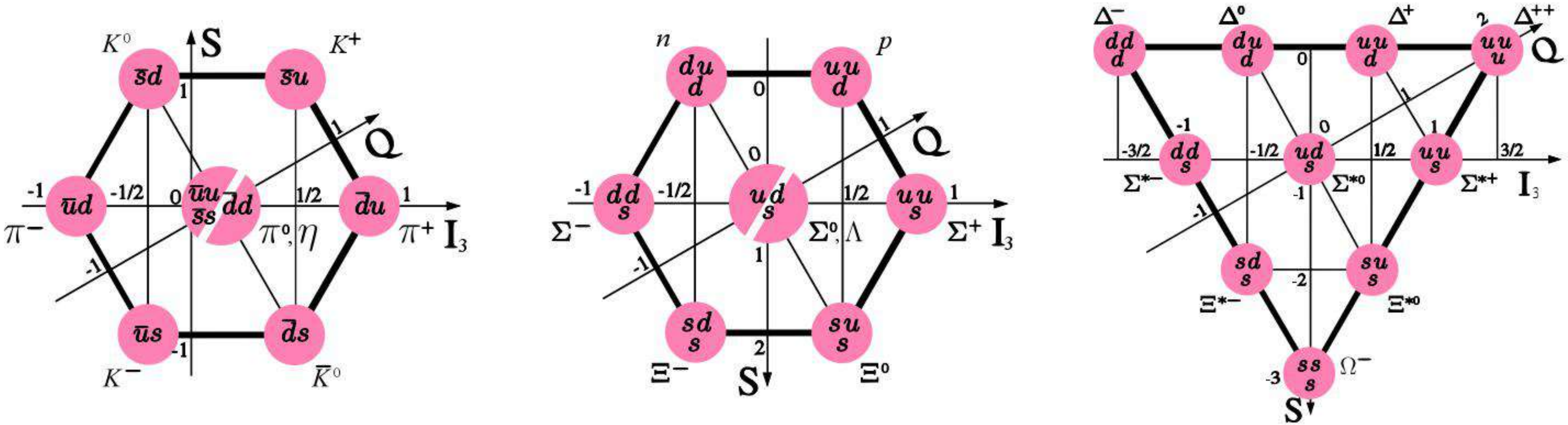
	RI @ 4 GeV	RGI	$\overline{\text{MS}}$ @ 2 GeV
m_s	96.4(1.1)(1.5)	127.3(1.5)(1.9)	95.5(1.1)(1.5)
m_{ud}	3.503(48)(49)	4.624(63)(64)	3.469(47)(48)
m_s/m_{ud}		27.53(20)(8)	
m_u	2.17(04)(10)	2.86(05)(13)	2.15(03)(10)
m_d	4.84(07)(12)	6.39(09)(15)	4.79(07)(12)

Relative contribution to total error:

	stat.	plateau	scale	mass	renorm.	cont.
m_s	0.702	0.148	0.004	0.064	0.061	0.691
m_{ud}	0.620	0.259	0.027	0.125	0.063	0.727
m_s/m_{ud}	0.921	0.200	0.078	0.125	—	0.301

(JHEP 1108:148,2011; PLB 701:265,2011)

Computing m_u and m_d



- Two sources of isospin breaking:
  - QCD: $\sim \frac{m_d - m_u}{\Lambda_{QCD}} \sim 1\%$
  - QED: $\sim \alpha(Q_u - Q_d)^2 \sim 1\%$
- On the lattice:
  - Include nondegenerate light quarks $m_u \neq m_d$
  - Include QED

Including isospin breaking on the lattice

$$S_{\mathrm{QCD+QED}} = S^{\mathrm{iso}}_{\mathrm{QCD}} + \frac{1}{2}(m_u - m_d)\int(\bar{u}u - \bar{d}d) + ie\int A_\mu j_\mu$$

with $j_\mu = \bar{q}Q\gamma_\mu q$

Method 1: operator insertion (RM123 '12-'13)

$$\langle\mathcal{O}\rangle = \langle\mathcal{O}\rangle^{\mathrm{iso}}_{\mathrm{QCD}} - \frac{1}{2}(m_u - m_d)\langle\mathcal{O}\int(\bar{u}u - \bar{d}d)\rangle^{\mathrm{iso}}_{\mathrm{QCD}} + \frac{1}{2}e^2\langle\mathcal{O}\int_{xy} j_\mu(x)D_{\mu\nu}(x-y)j_\nu(y)\rangle^{\mathrm{iso}}_{\mathrm{QCD}} + \ldots$$

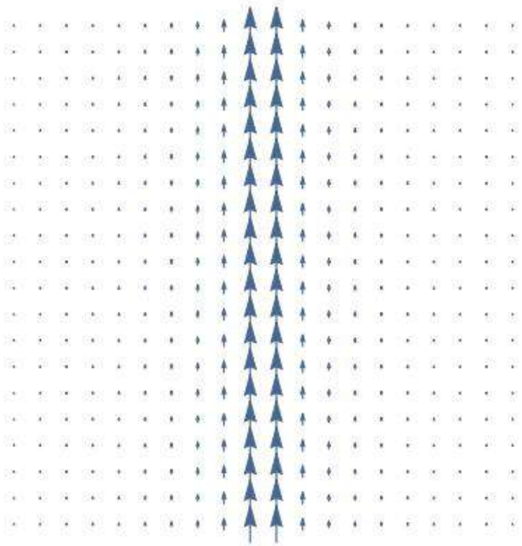
Method 2: direct calculation

(Eichten '97, Blum et al '07-, BMWc '10-, MILC '09, Blum et al '10, RBC/UKQCD '12, QCDSF '15, Giusti et. al. '15. . .)

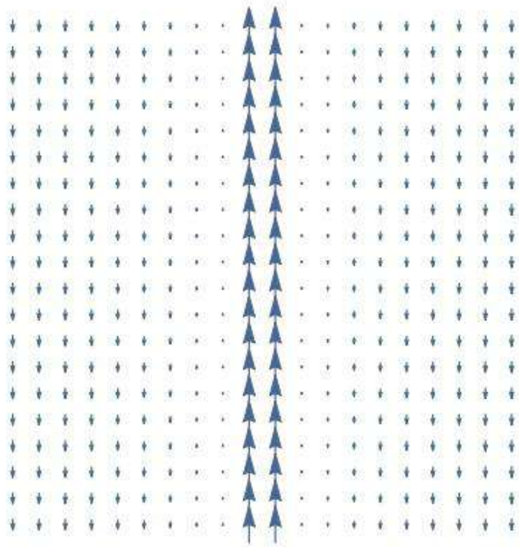
Challenges of QED simulations

- Effective theory only (UV completion unclear)
- π^+, p, etc. no more gauge invariant
- QED (additive) mass renormalization
- Power law FV effects (soft photons)

Zero mode of gauge potential unconstrained by action



Remove $\vec{p} = 0$ modes in fixed gauge(Hayakawa, Uno, 2008)



QED ACTION

QED is an Abelian gauge theory with no self-interaction

- Compactifying QED induces spurious self-interaction

➢ Keep it non-compact (no problem with topology in 4D-$U(1)$)

- Need signals for gauge dependent objects

➢ insert gauge links or gauge fixing

$$S_{\text{QED}} = \frac{1}{2V_4} \sum_{\mu,k} |\hat{k}|^2 |A_\mu^k|^2 \quad \text{with} \quad \hat{k}_\mu = \frac{e^{iak_\mu} - 1}{ia}$$

- Momentum modes decouple ➢ quenched theory trivial

Finite volume gauge symmetry

- Periodicity requirement from gauge field

$$A_\mu(x) \to A_\mu(x) + \frac{1}{e}\partial_\mu \Lambda(x) \implies \partial_\mu \Lambda(x) = \partial_\mu \Lambda(x+L)$$

- is loser than from fermion field

$$\psi(x) \to e^{-i\Lambda(x)}\psi(x), \quad \bar{\psi}(x) \to \psi(x) e^{i\Lambda(x)} \implies \Lambda(x) = \Lambda(x+L)$$

- Fermionic action not invariant under GT

$$\Lambda(x) = c_\mu x^\mu \implies \delta\mathcal{L} = i\bar{\psi}(\gamma^\mu \partial_\mu \Lambda)\psi = ic_\mu \bar{\psi}\gamma^\mu \psi$$

- Add source term to action to restore gauge invariance

$$\mathcal{L}_{\text{src}} = J_\mu \bar{\psi}\gamma^\mu \psi \qquad J_\mu \to J_\mu - ic_\mu$$

QED in finite volume

- Gauge invariant definition of no external source:

$$\frac{e}{V_4}\int d^4x A_\mu(x) + iJ_\mu = 0$$

with partial gauge fixing $J_\mu = 0$ ➛ $\mathrm{QED_{TL}}$

- Imposing electric flux neutrality per timeslice:

$$\frac{e}{V_3}\int d^3x A_i(t,\vec{x}) = 0$$

with partial gauge fixing $A_0(t,\vec{p}=0) = 0$ ➛ $\mathrm{QED_L}$

Momentum subtraction

- Removing momentum modes with measure 0 as $V \to \infty$ allowed
- Remove $k = 0$ from momentum sum (QED_{TL})
  - Realised by a constraint term in the action

$$\lim_{\xi \to 0} \frac{1}{\xi} \left(\int d^4x A_\mu(x) \right)^2$$

  - Couples all times ➛ no transfer matrix!
- Remove $\vec{k} = 0$ from momentum sum (QED_L)
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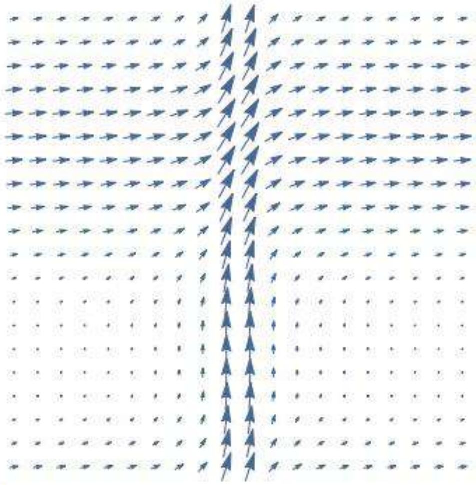
$$\lim_{\xi(t) \to 0} \int dt \frac{1}{\xi(t)} \left(\int d^3x A_\mu(x) \right)^2$$

  - Transfer matrix exists



- Gauge fields unaffected in QED_{TL}, only Polyakov loops

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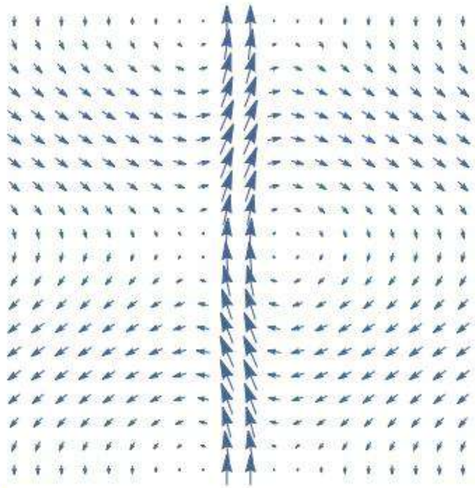

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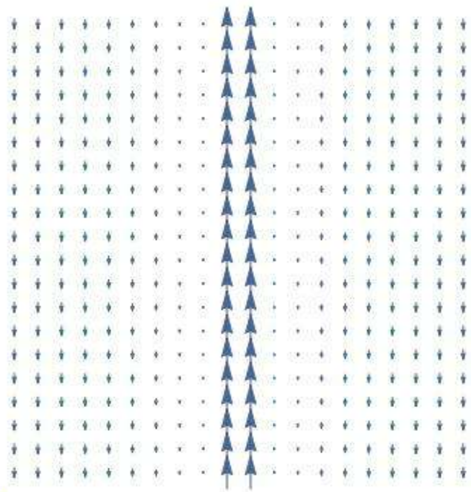

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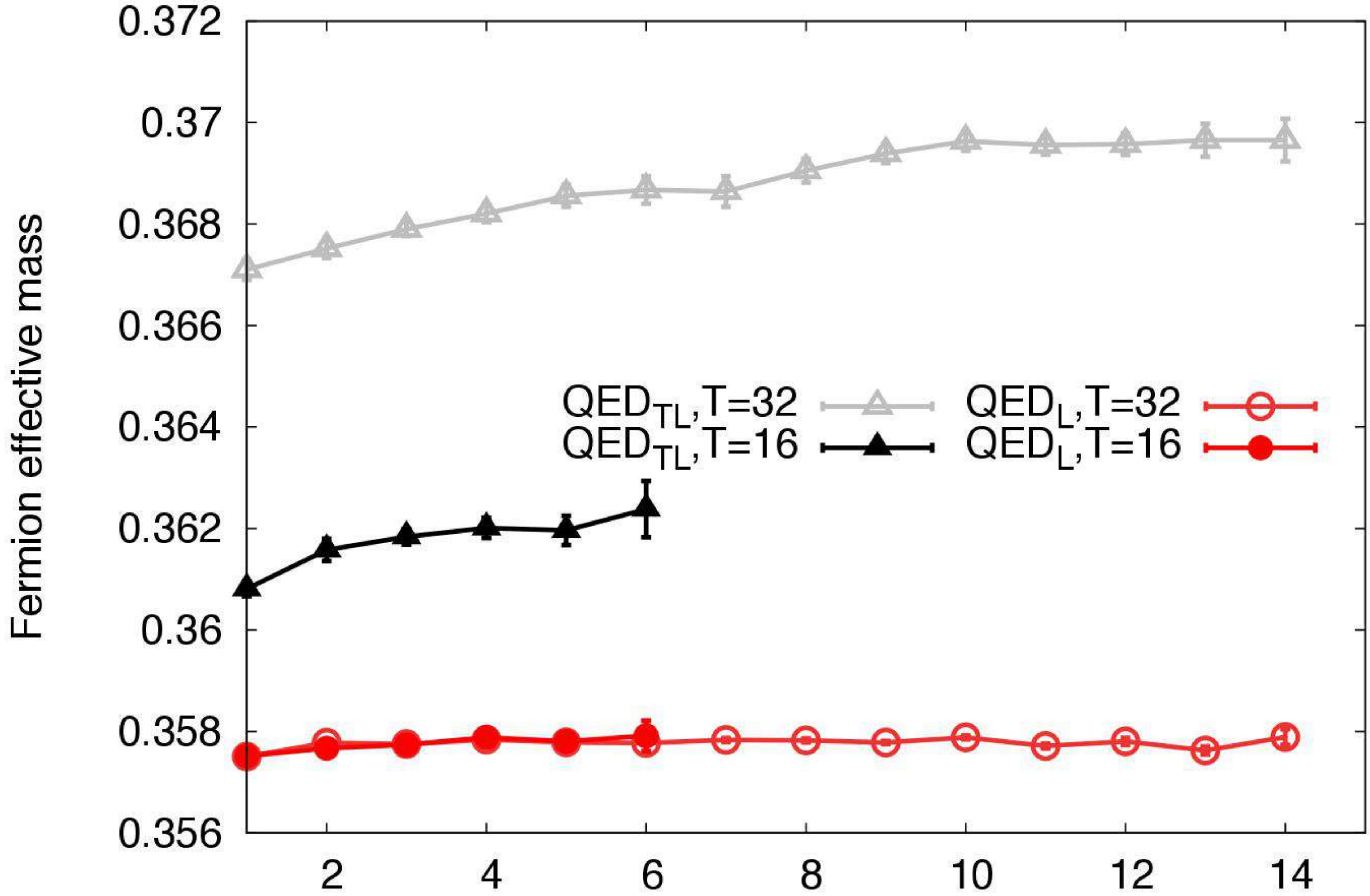
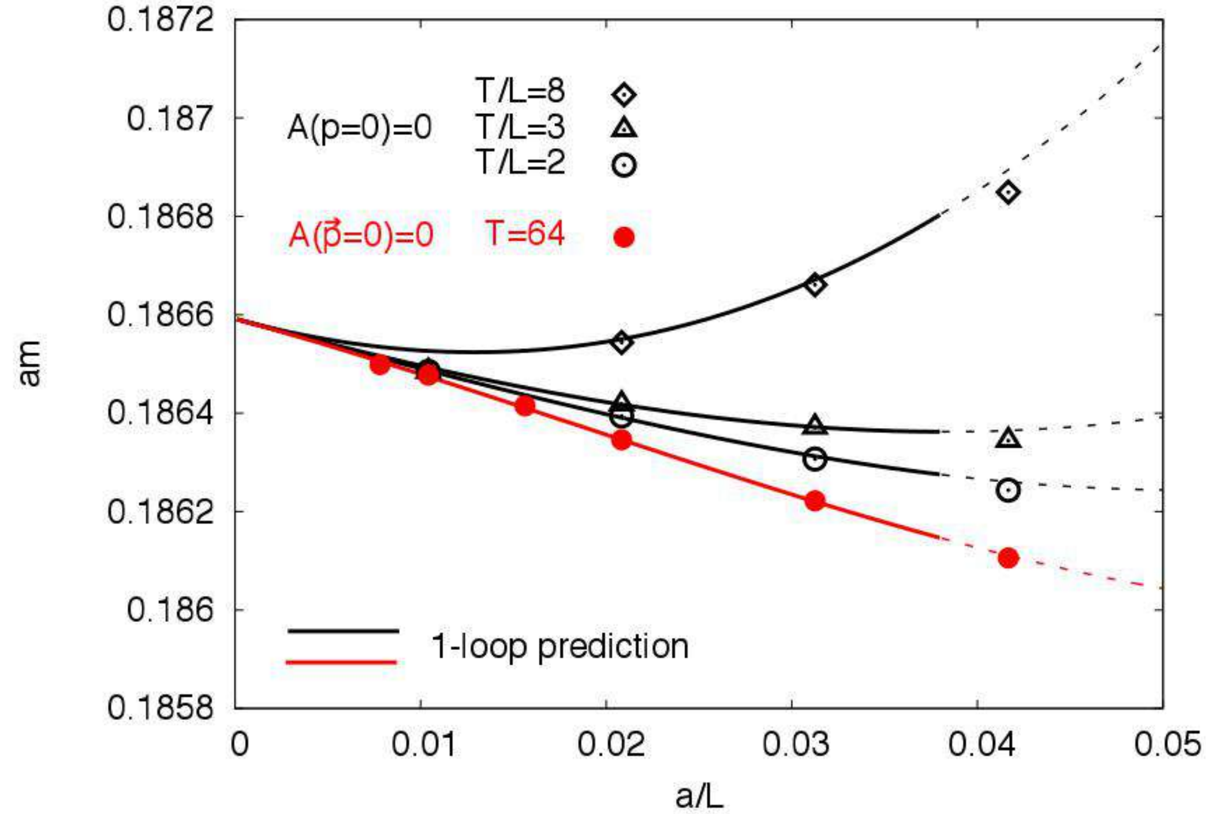
Quenched QED FV effects



Finite volume subtraction

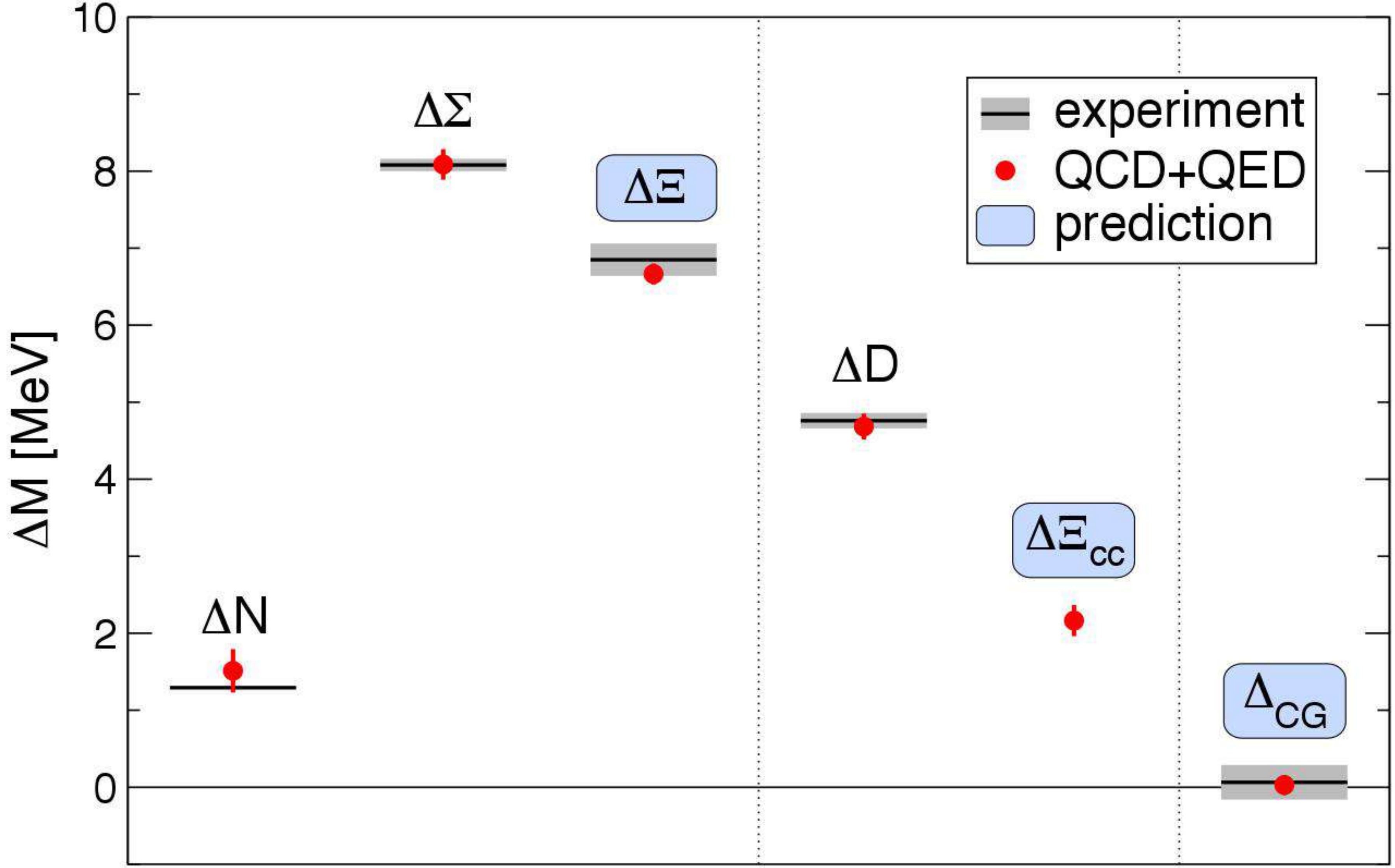
- Universal to $O(1/L^2)$
- Compositmess at $1/L^3$
- Fit $O(1/L^3)$
- Divergent T dependence for $p = 0$ mode subtraction
- No T dependence for $\vec{p} = 0$ mode subtraction



$$\delta m = q^2\alpha\left(\frac{\kappa}{2mL}\left(1+\frac{2}{mL}-\frac{3\pi}{(mL)^3}\right)\right)$$

(BMWc, 2014)

Hadronic isospin splitting



(BMWc 2014)

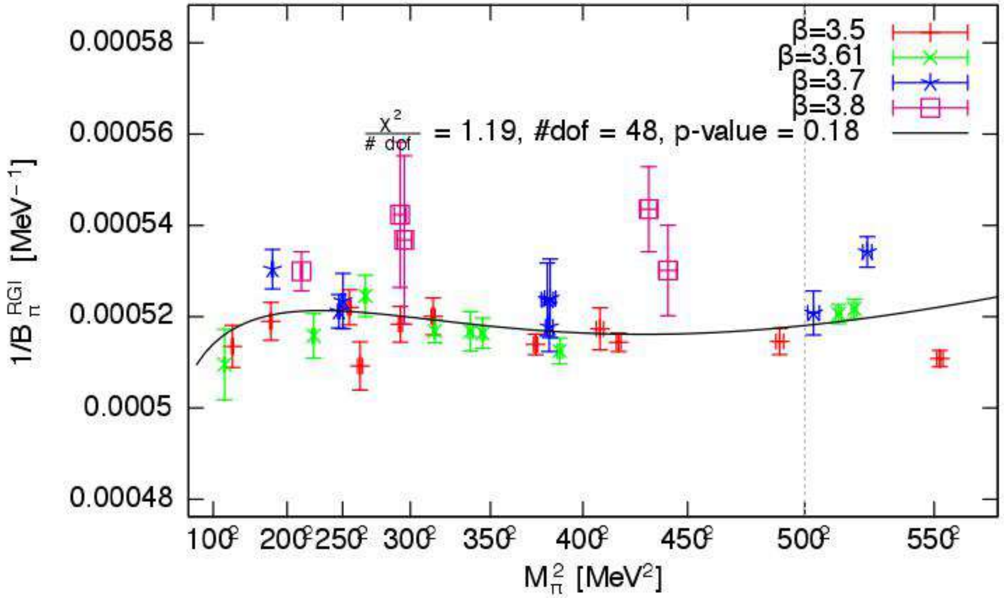
Masses of the *u* and *d* quarks

Goal:

- Directly compute m_u and m_d

Method:

- Results in qQED as a first step
- Direct calculation in full QED difficult



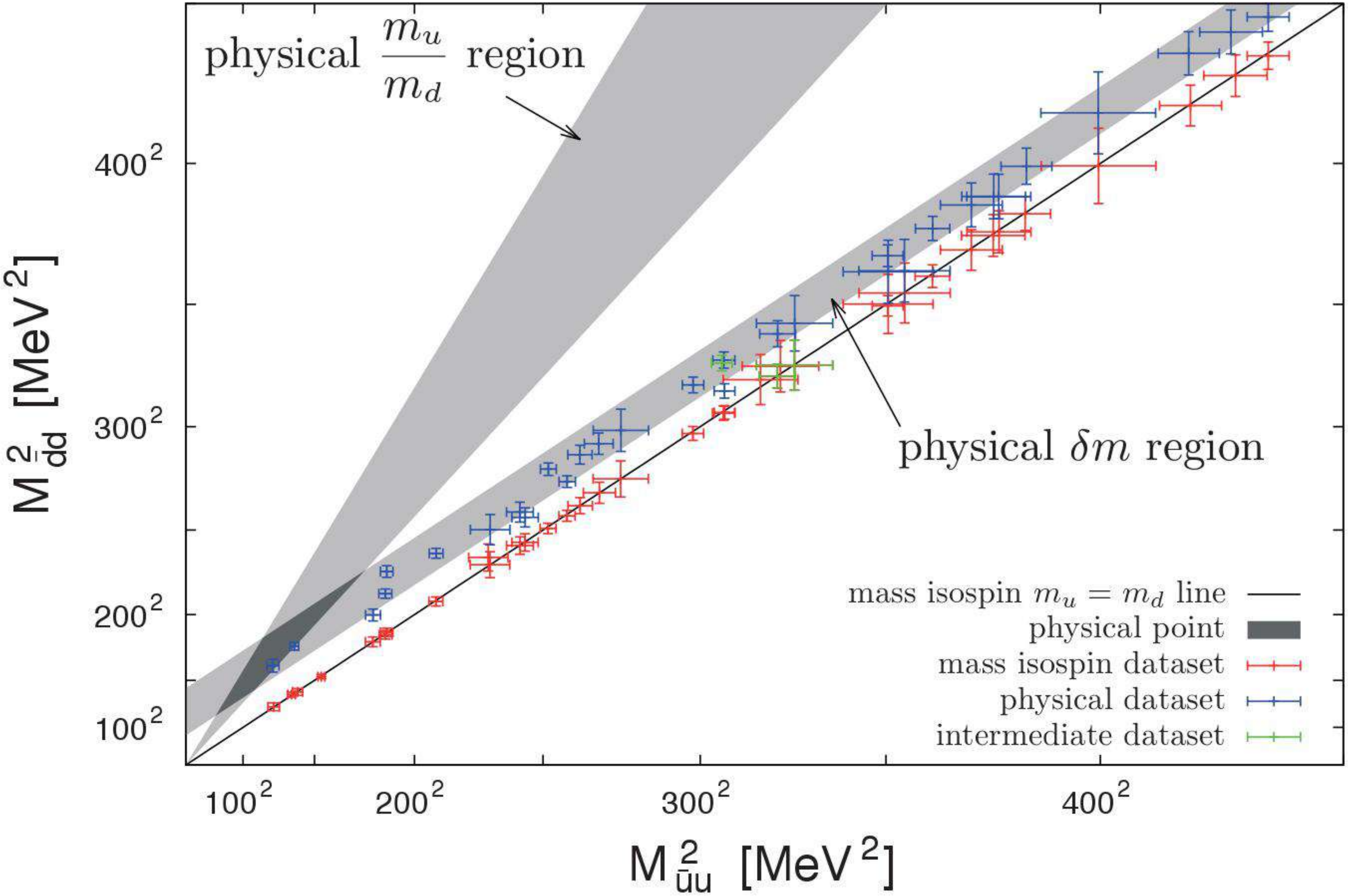
Computing $m_u - m_d$:

- Parameterize $\delta m = m_u - m_d$ via $\Delta M^2 = M_{uu}^2 - M_{dd}^2$

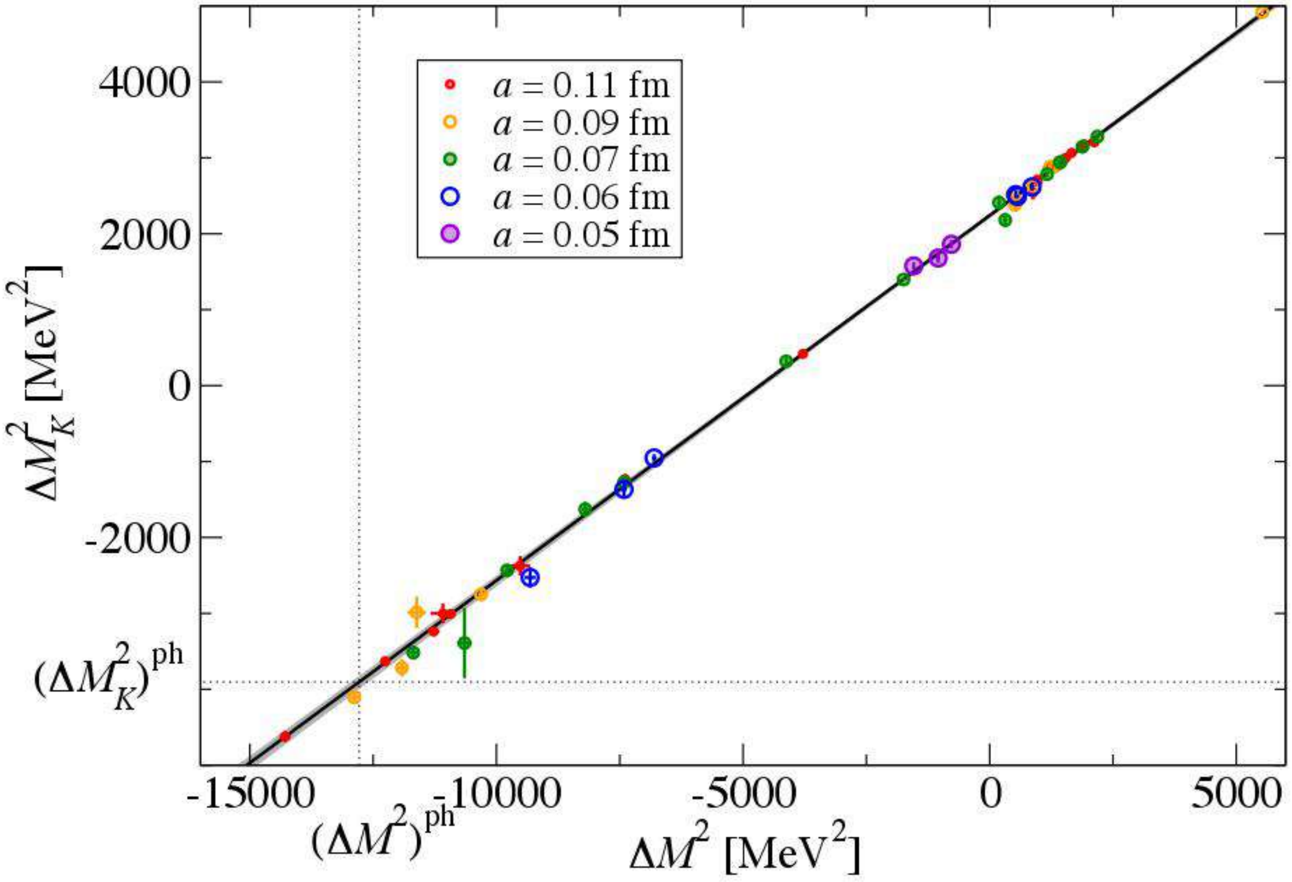
$$\Delta M^2 = 2B_2\delta m + O(m_{ud}\alpha, m_{ud}\delta m, \alpha^2, \alpha\delta m, \delta m^2)$$

- Power counting: $O(\delta m) = O(m_{ud})$
- Condensate parameter $B_2^{\overline{MS}}(2\text{GeV}) = 2.85(7)(2)\text{GeV}$ (BMWc 2013)

Our dataset


physical $\frac{m_u}{m_d}$ region
physical δm region
mass isospin $m_u = m_d$ line
physical point
mass isospin dataset
physical dataset
intermediate dataset
100^2
200^2
300^2
400^2
$M^2_{\bar{d}d}$ [MeV^2]
$M^2_{\bar{u}u}$ [MeV^2]

Extracting physical ΔM^2

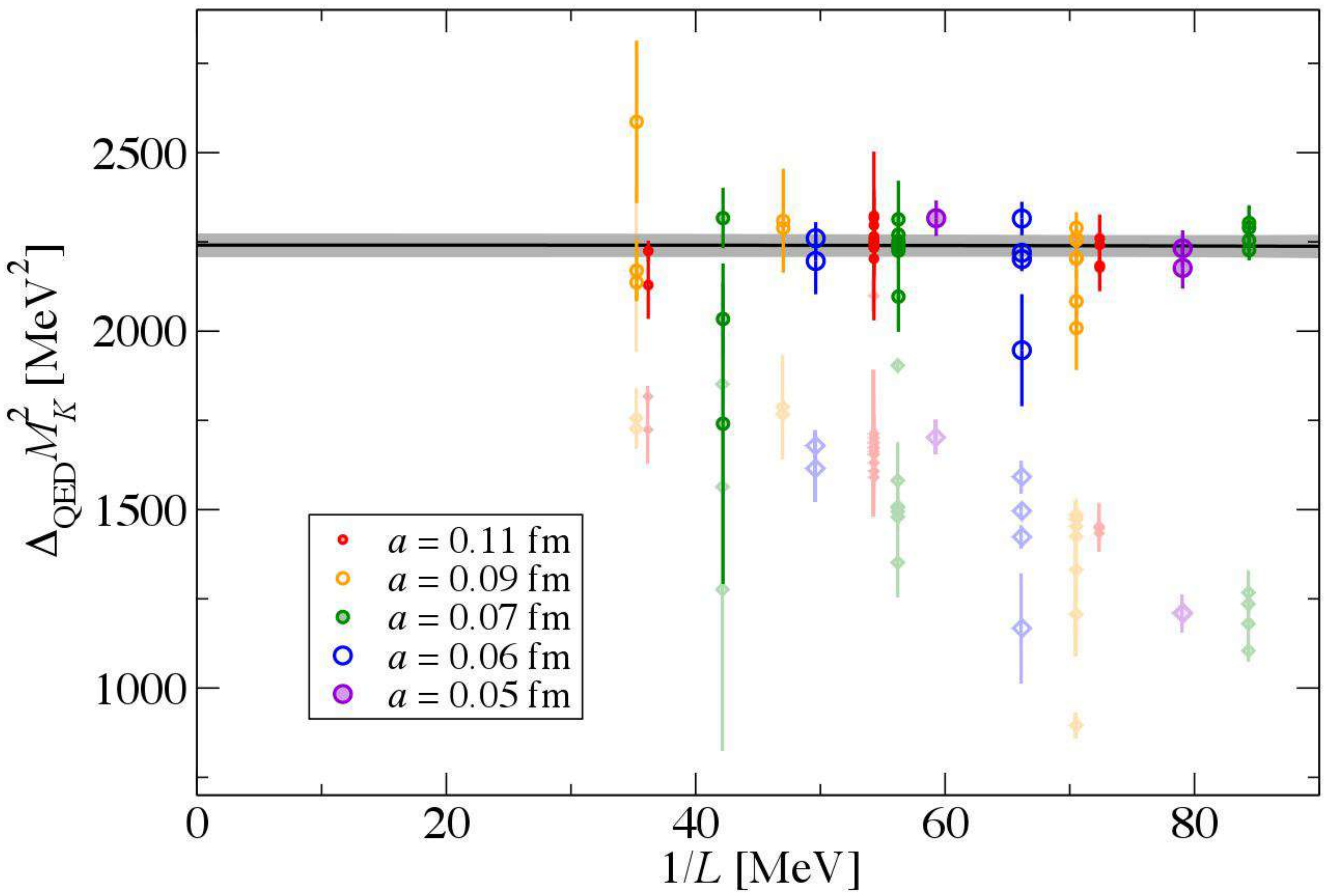


$$\Delta M_K^2 = \Delta M^2 C_X + \alpha D_X$$

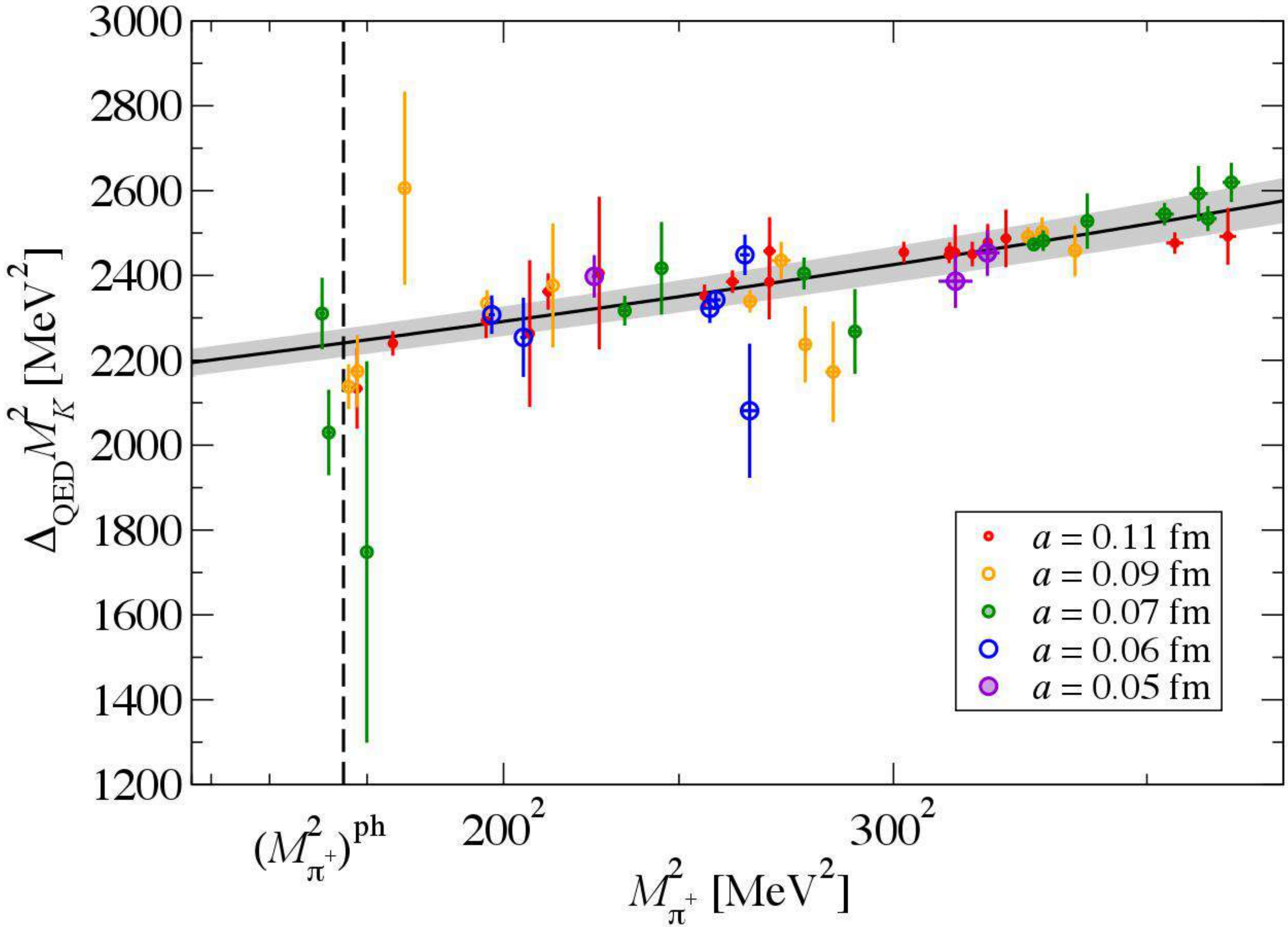
$$C_X = c_X^0 + c_X^1 \hat{M}_\pi^2 + c_X^2 \hat{M}_K^2 + c_X^3 f(a)$$

$$D_X = d_X^0 + d_X^1 \hat{M}_\pi^2 + d_X^2 \hat{M}_K^2 + d_X^3 a + d_X^4 \frac{1}{L^3}$$

Finite volume



Chiral interpolation



Results

- $\delta m^{\overline{MS}}(2\text{GeV}) = -2.41(6)(4)(9)\text{MeV}$
- $m_u^{\overline{MS}}(2\text{GeV}) = 2.27(6)(5)(4)\text{MeV}$
- $m_d^{\overline{MS}}(2\text{GeV}) = 4.67(6)(5)(4)\text{MeV}$
- $m_u/m_d = 0.485(11)(8)(14)$

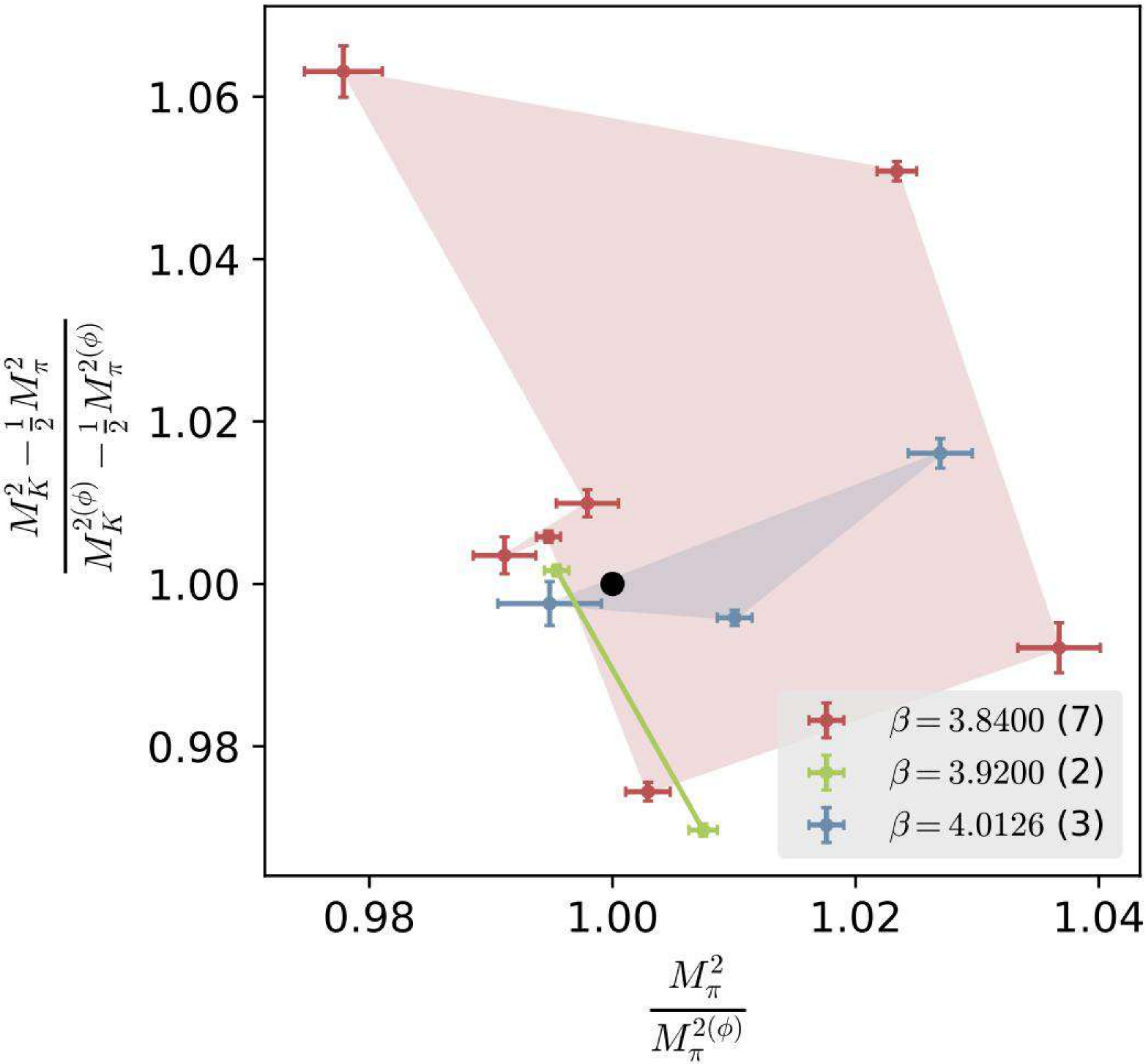
- $\epsilon := \frac{\Delta_{\text{QED}} M_K^2 - \Delta_{\text{QED}} M_\pi^2}{\Delta M_\pi^2} = 0.73(2)(5)(17)(2)$
- $R := \frac{m_s - m_{ud}}{m_d - m_u} = 38.2(1.1)(0.8)(1.4)$
- $Q := \sqrt{\frac{m_s^2 - m_{ud}^2}{m_d^2 - m_u^2}} = 23.4(0.4)(0.3)(0.4)$

(BMWc, 2016)

Motivation

Why staggered?

- Staggered is much faster!
- ☞ Allows smaller m_q, directly bracket physical point
- ☞ Allows large volumes $L > 6\mathrm{fm}$ (FV effects negligible$\ll 1‰$)
- Better continuum behaviour ($O(\alpha a^2)$)
- No additive mass renormalization
- We only need pseudoscalar mesons
- 4 step stout smeared $N_f = 2 + 1 + 1$
- Scale setting with f_π (m_s/m_{ud} very insensitive)



4 stout smeared
$N_f = 2 + 1 + 1$
staggered
ensembles

Meson mass extraction

Extracting staggered meson masses:

- Multi-state fit
- Time-shifted propagator

Basic idea: staggered propagator for $m(T/2 - t) \ll 1$

$$c_t = e^{-mt}(c_0 + (-1)^t c_1 e^{-\Delta t})$$

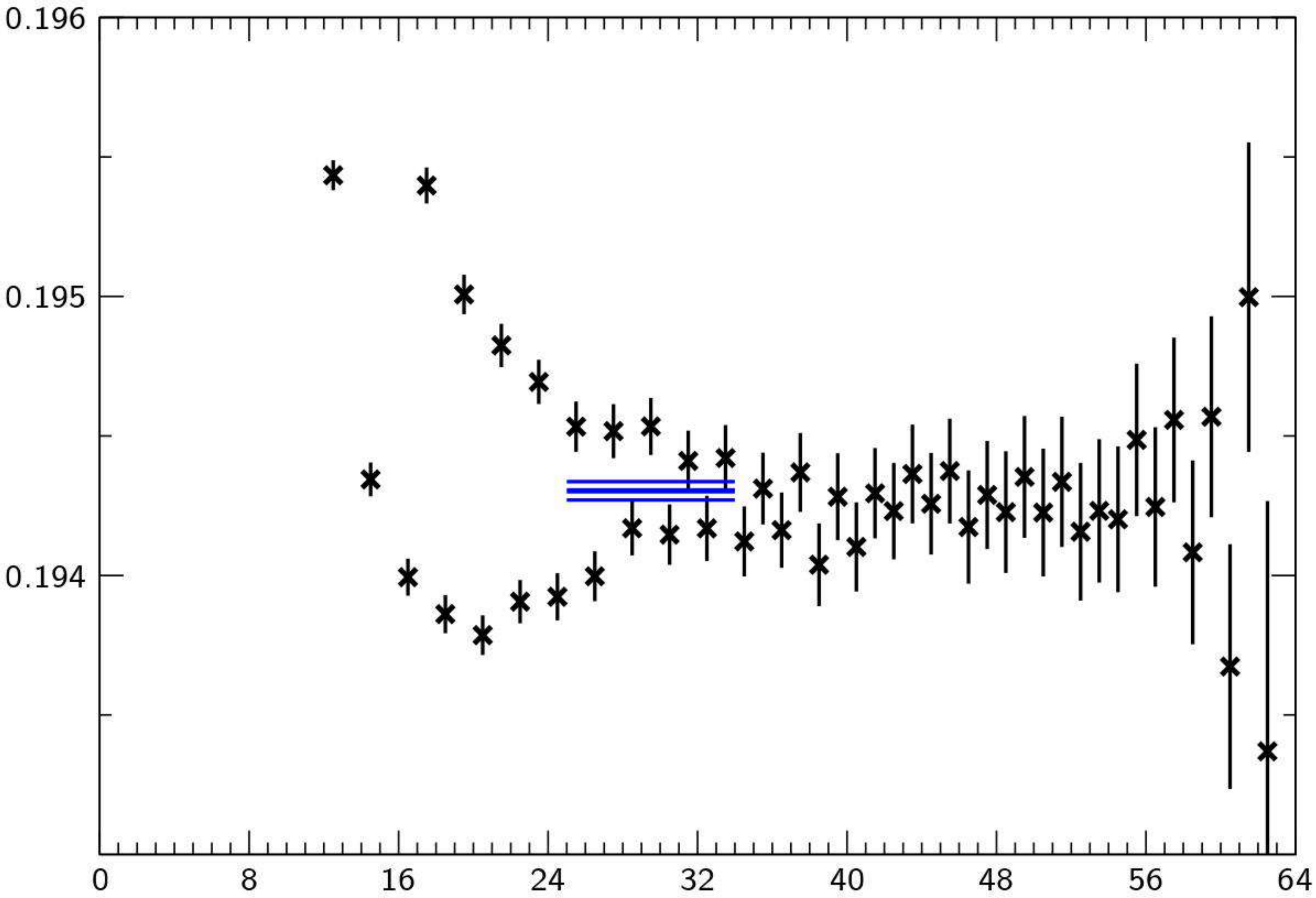
define time shifted propagator

$$d_t := c_t + e^{m+\Delta} c_{t+1}$$

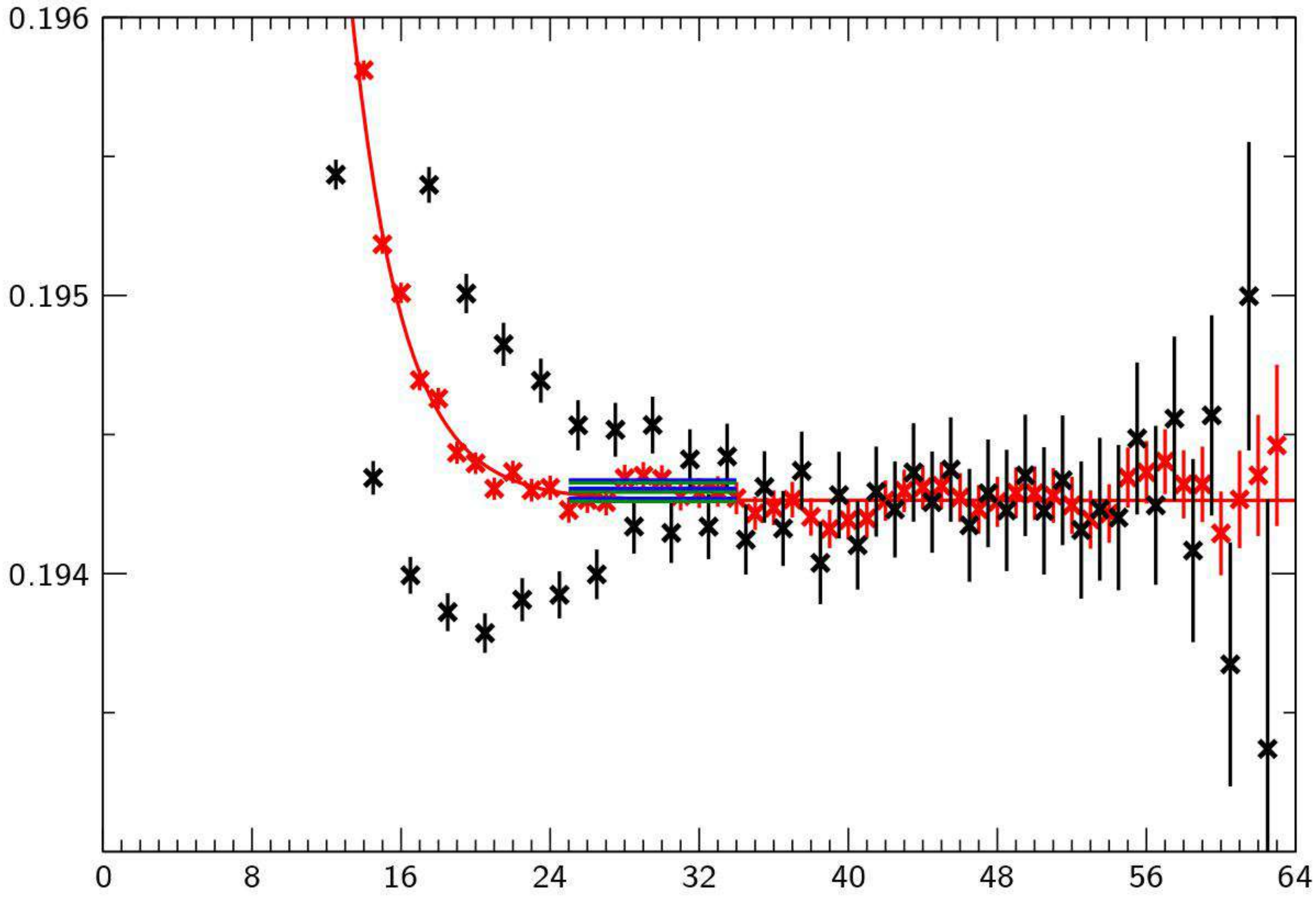
Determine Δ by minimizing effective mass fluctuations

- Cross-checked with variational multi-state fit

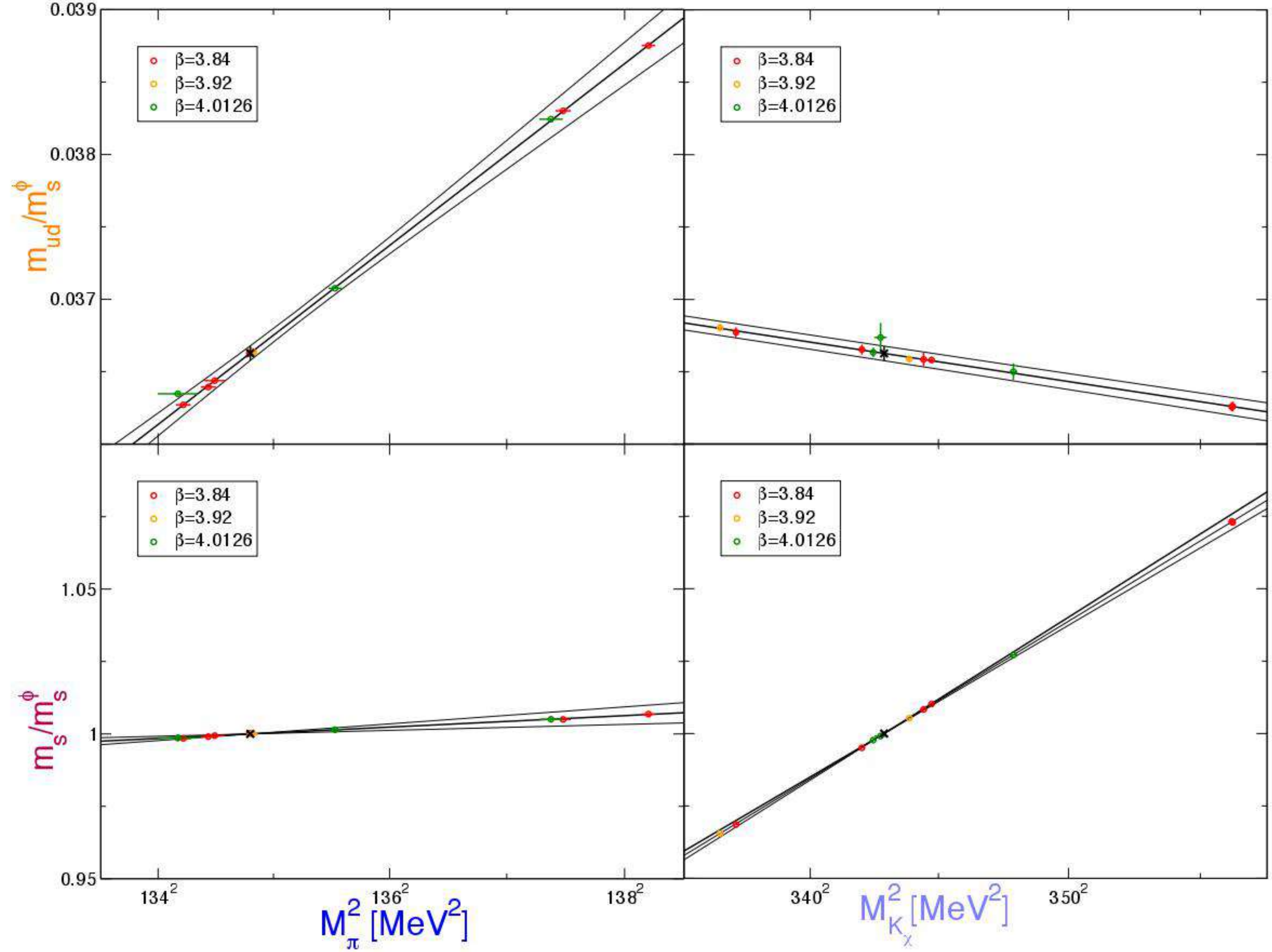
Meson mass extraction



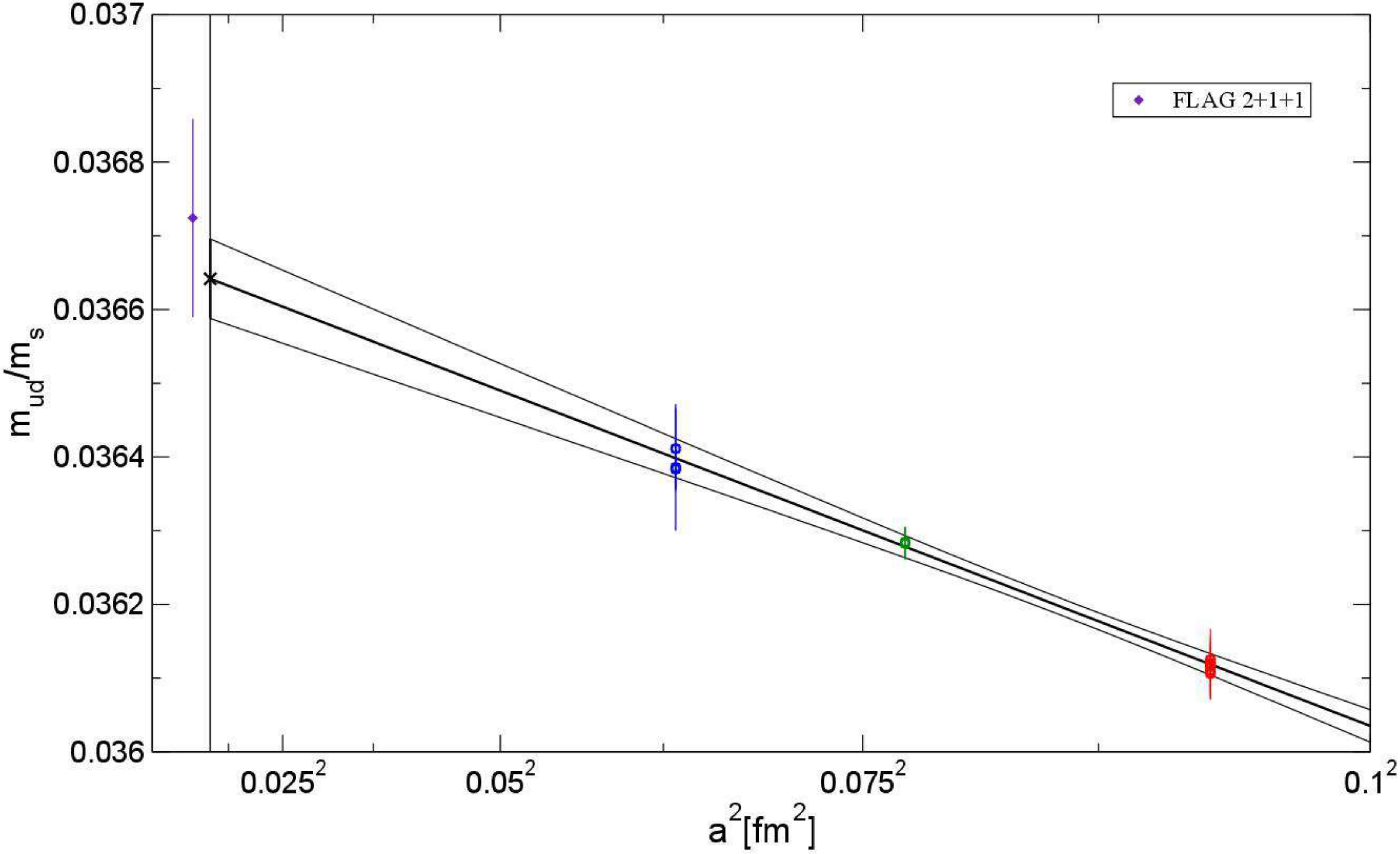
Meson mass extraction



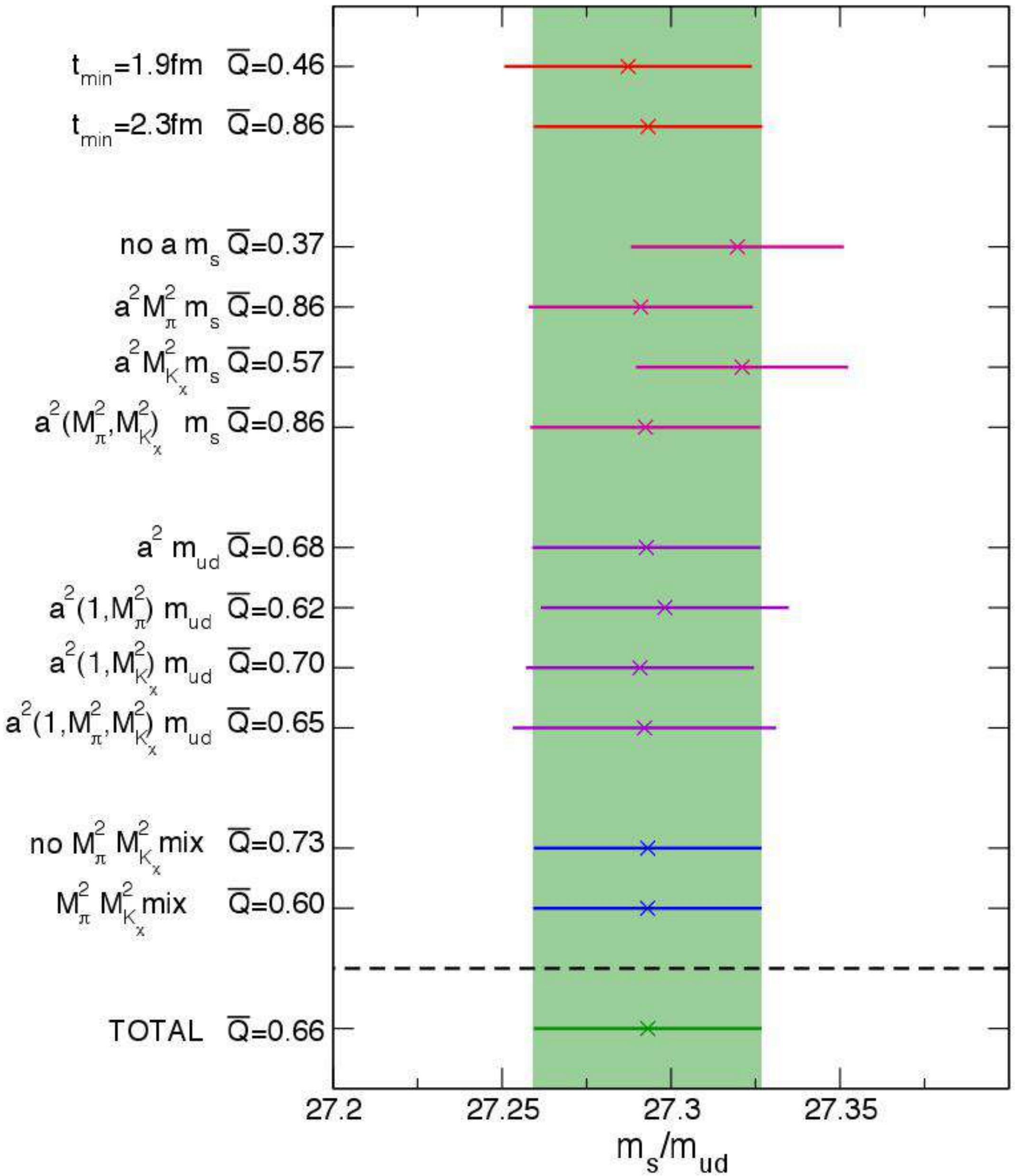
Physical point interpolation



Continuum extrapolation



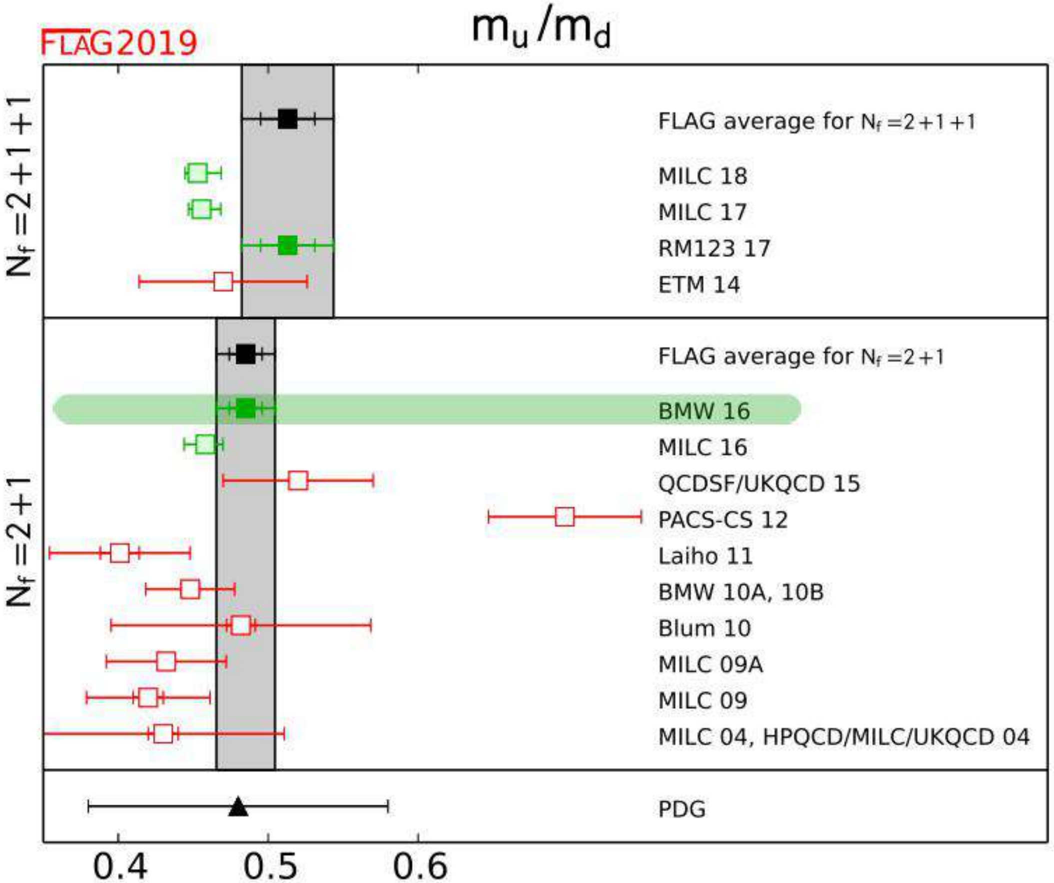
Systematic error

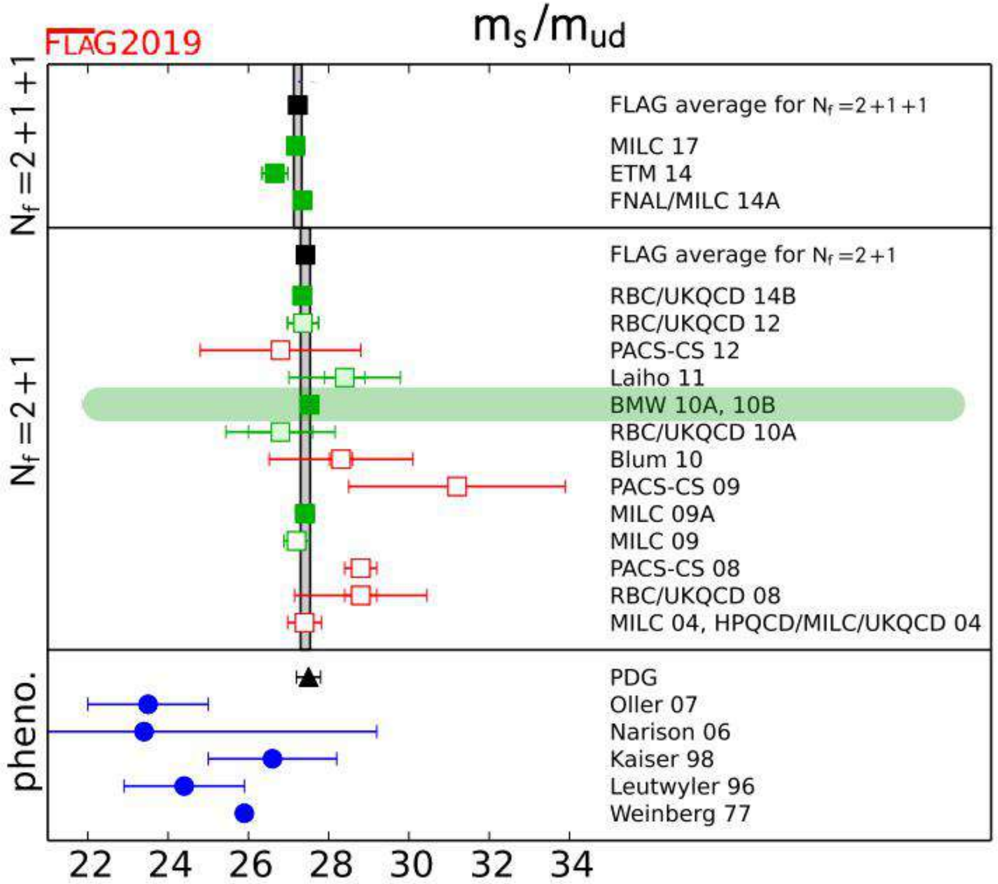


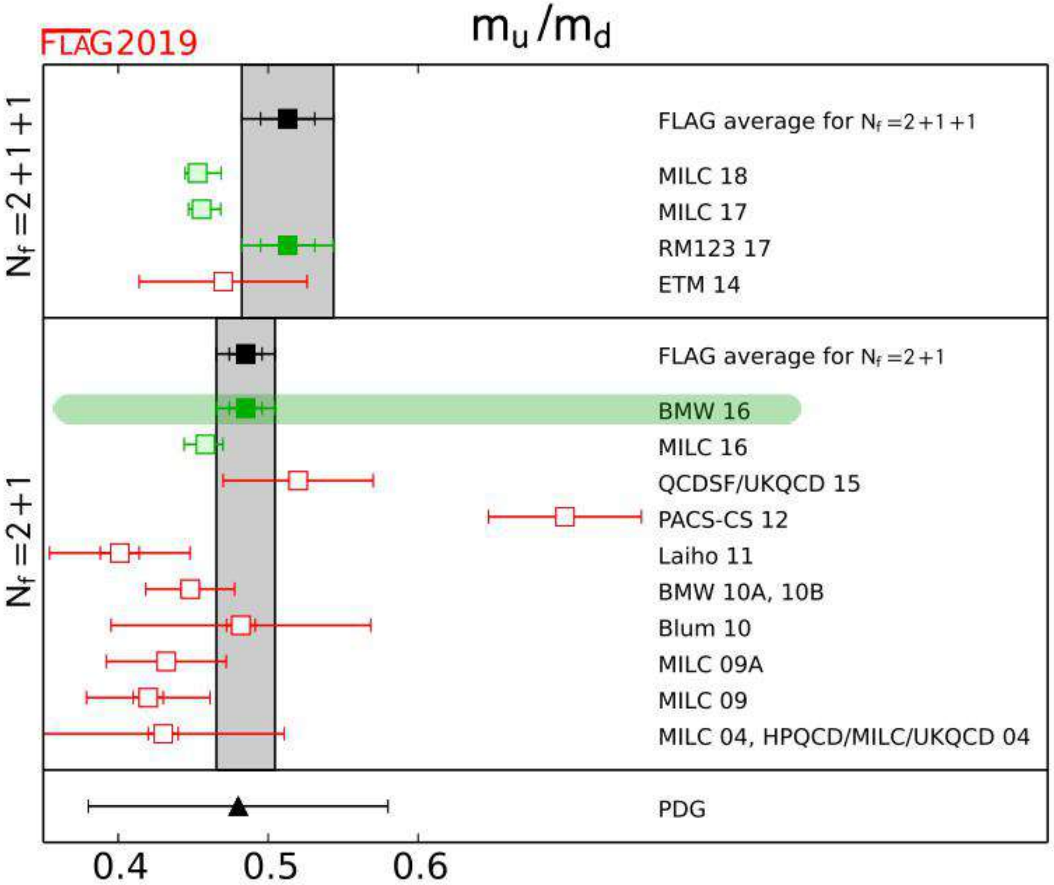
- 64 variations of analysis:
  - 2 plateaux ranges
  - 4 m_s continuum terms
  - 4 m_{ud} continuum terms
  - 2 χ interpolation mixing
- Other variations crosschecked: no further relevant terms found

Final result:

$$\frac{m_s}{m_{ud}} = 27.293(33)(8)$$


FLAG2019
m_u/m_d
$N_f=2+1+1$
$N_f=2+1$
FLAG average for $N_f=2+1+1$
MILC 18
MILC 17
RM123 17
ETM 14
FLAG average for $N_f=2+1$
BMW 16
MILC 16
QCDSF/UKQCD 15
PACS-CS 12
Laiho 11
BMW 10A, 10B
Blum 10
MILC 09A
MILC 09
MILC 04, HPQCD/MILC/UKQCD 04
PDG
0.4
0.5
0.6


FLAG2019
m_s/m_{ud}
$N_f=2+1+1$
$N_f=2+1$
pheno.
FLAG average for $N_f=2+1+1$
MILC 17
ETM 14
FNAL/MILC 14A
FLAG average for $N_f=2+1$
RBC/UKQCD 14B
RBC/UKQCD 12
PACS-CS 12
Laiho 11
BMW 10A, 10B
RBC/UKQCD 10A
Blum 10
PACS-CS 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
MILC 04, HPQCD/MILC/UKQCD 04
PDG
Oller 07
Narison 06
Kaiser 98
Leutwyler 96
Weinberg 77
22
24
26
28
30
32
34


FLAG2019
m_u/m_d
$N_f = 2+1+1$
FLAG average for $N_f = 2+1+1$
MILC 18
MILC 17
RM123 17
ETM 14
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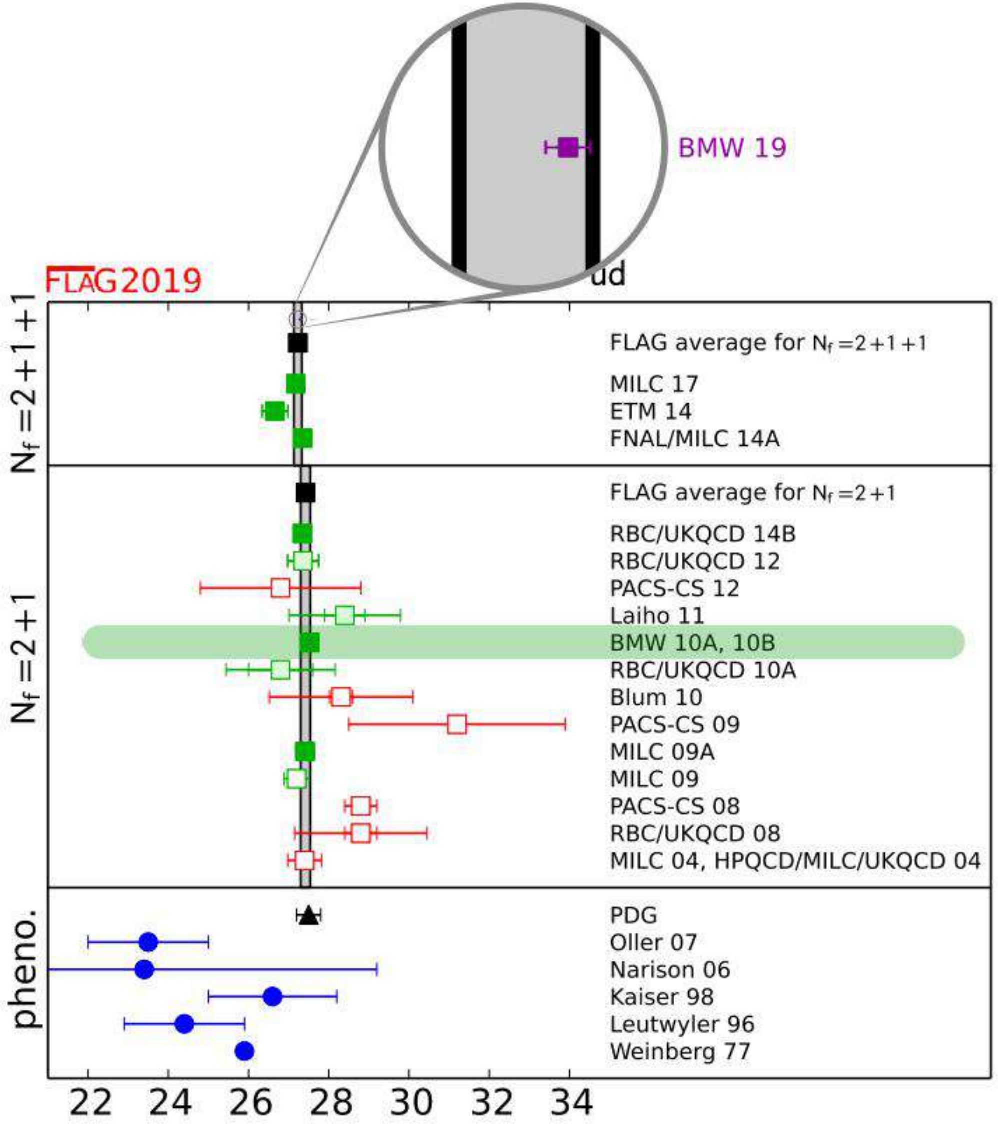
FLAG average for $N_f = 2+1$
BMW 16
MILC 16
QCDSF/UKQCD 15
PACS-CS 12
Laiho 11
BMW 10A, 10B
Blum 10
MILC 09A
MILC 09
MILC 04, HPQCD/MILC/UKQCD 04
PDG
0.4
0.5
0.6


BMW 19
FLAG2019
ud
$N_f = 2+1+1$
FLAG average for $N_f = 2+1+1$
MILC 17
ETM 14
FNAL/MILC 14A
$N_f = 2+1$
FLAG average for $N_f = 2+1$
RBC/UKQCD 14B
RBC/UKQCD 12
PACS-CS 12
Laiho 11
BMW 10A, 10B
RBC/UKQCD 10A
Blum 10
PACS-CS 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
MILC 04, HPQCD/MILC/UKQCD 04
pheno.
PDG
Oller 07
Narison 06
Kaiser 98
Leutwyler 96
Weinberg 77
22
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32
34

BACKUP

Action details

Goal:

- Optimize physics results per CPU time
- Conceptually clean formulation

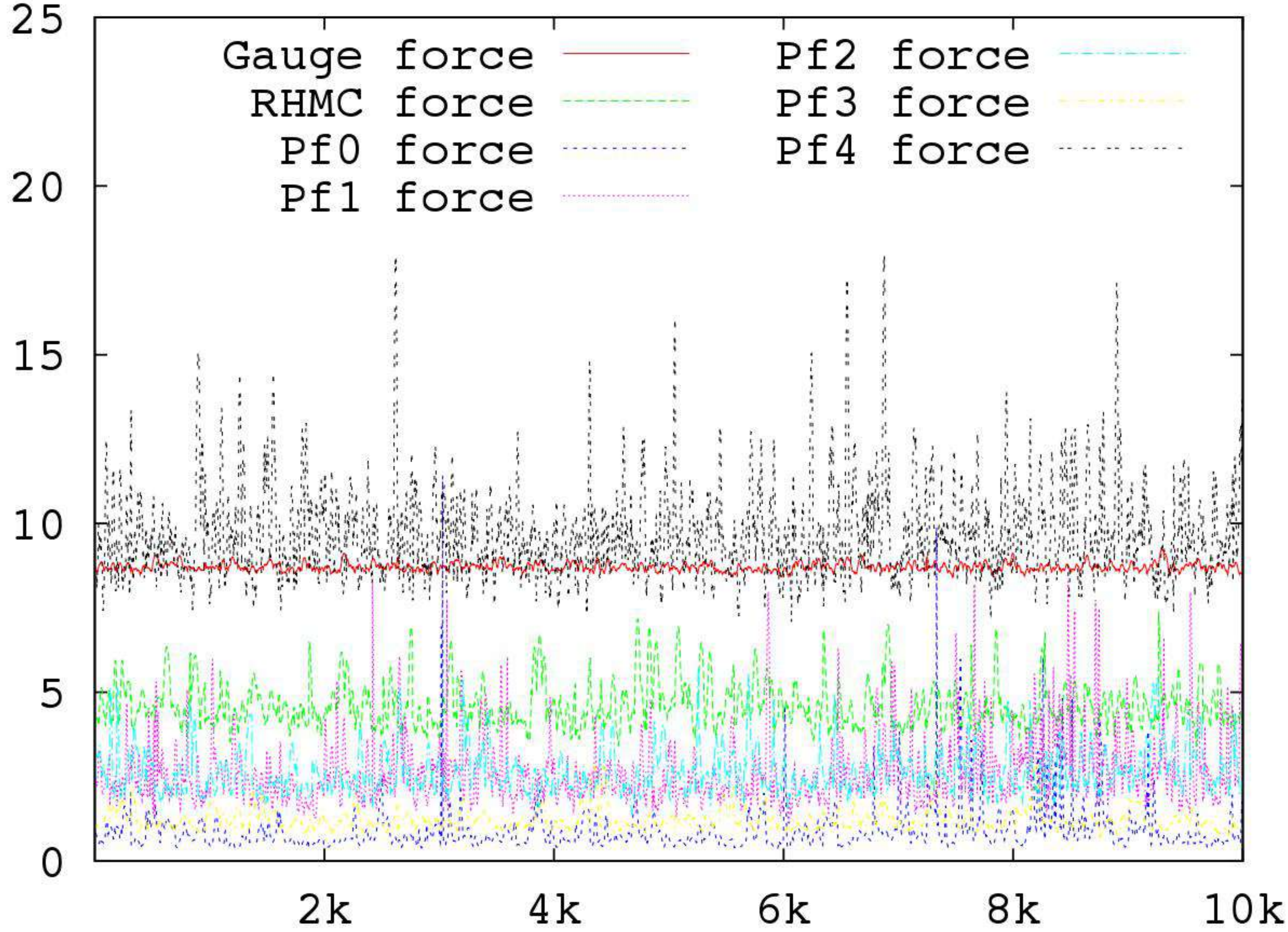
Method:

- 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)

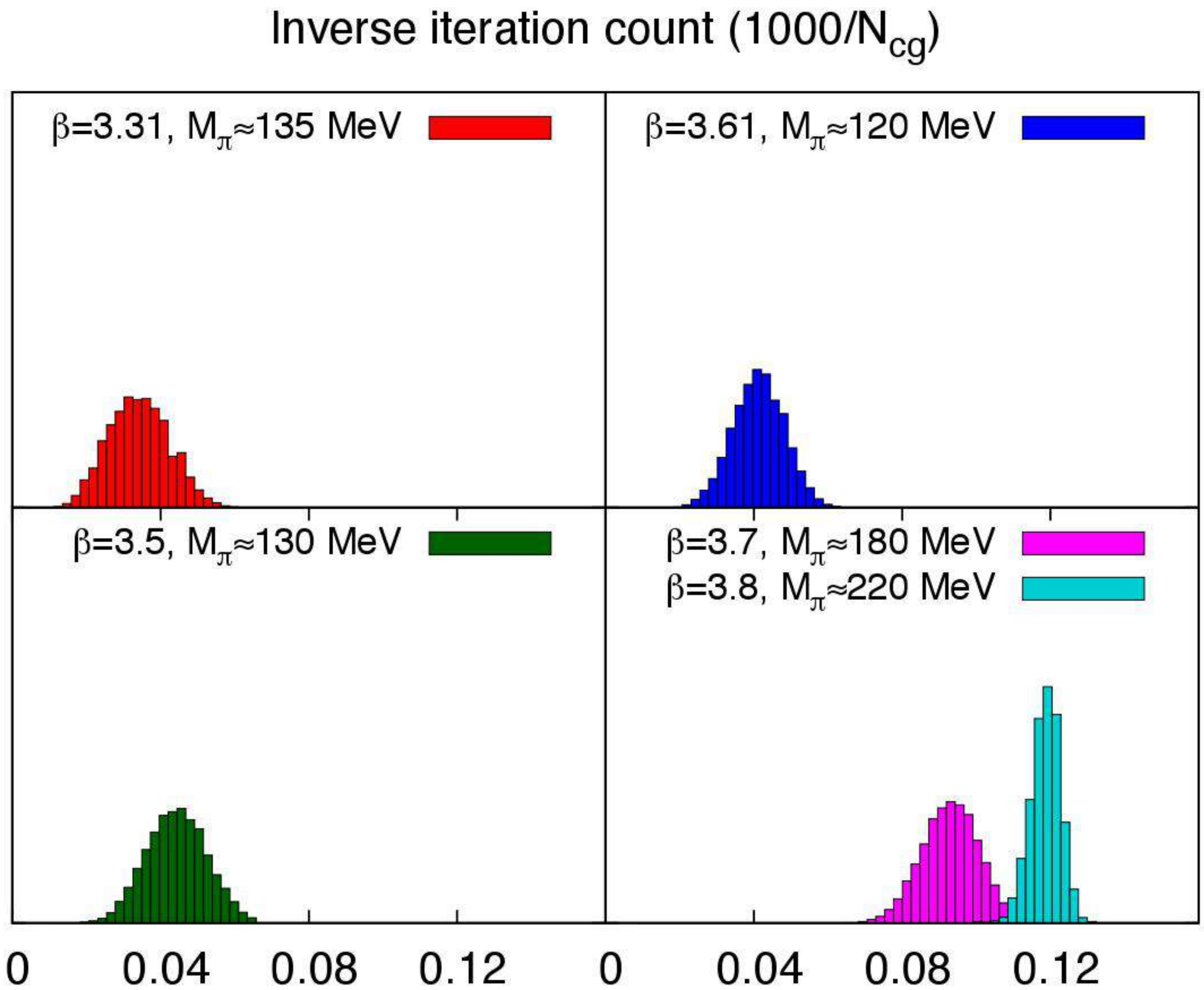
➢ Discretization effects of $O(\alpha_s a, a^2)$

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

Algorithm stability

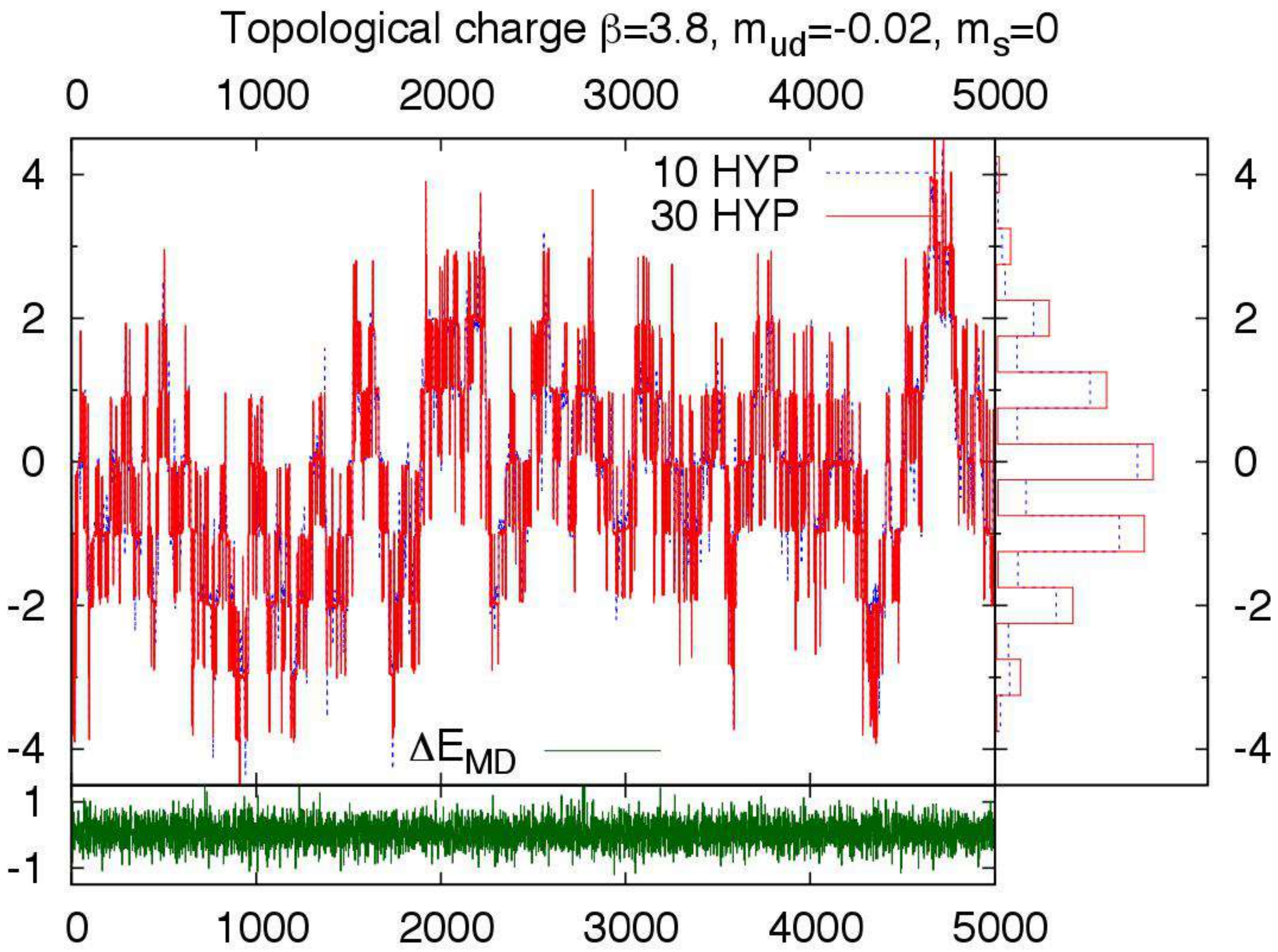


No exceptional configs



Topological sector sampling

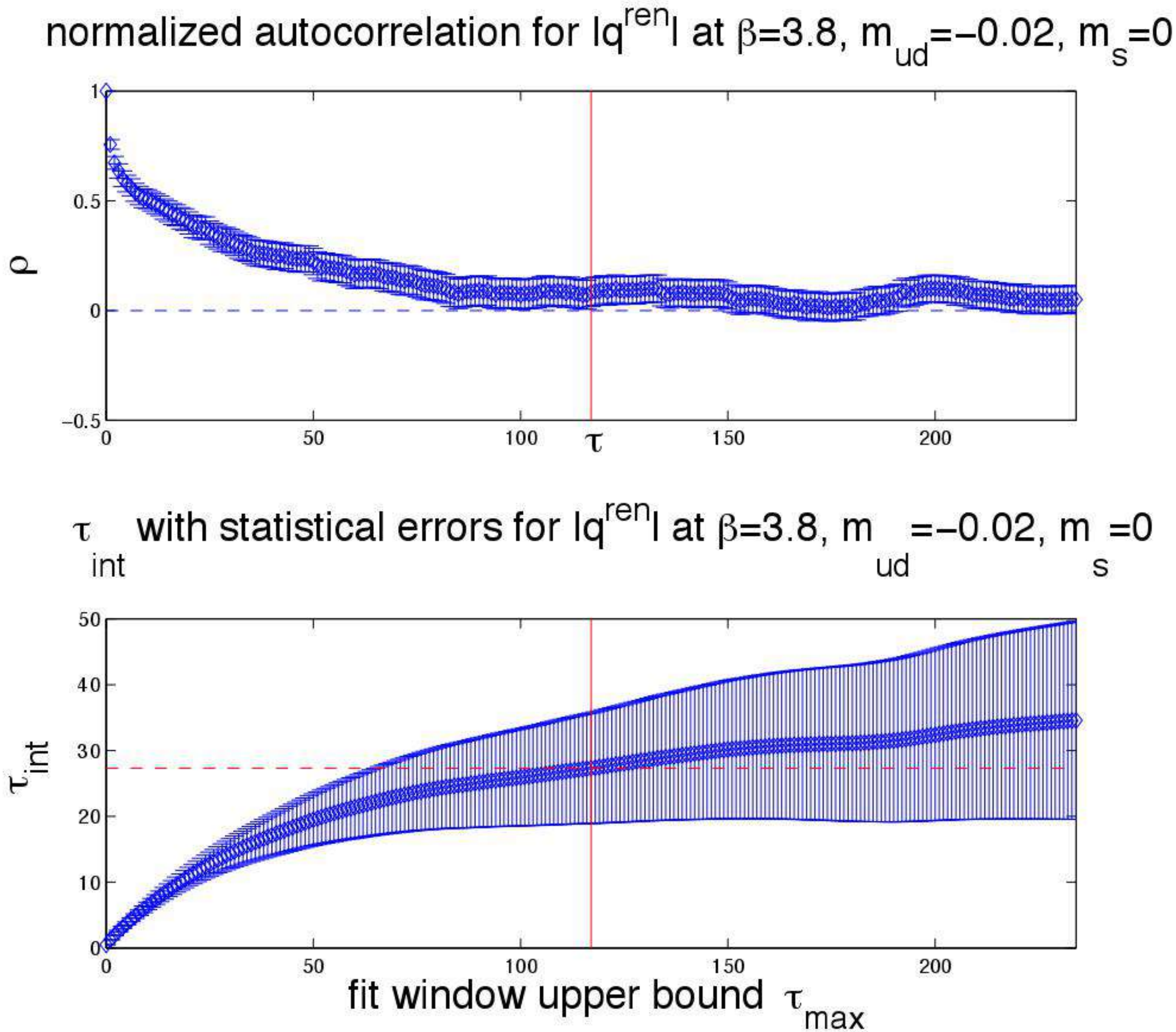
worst case



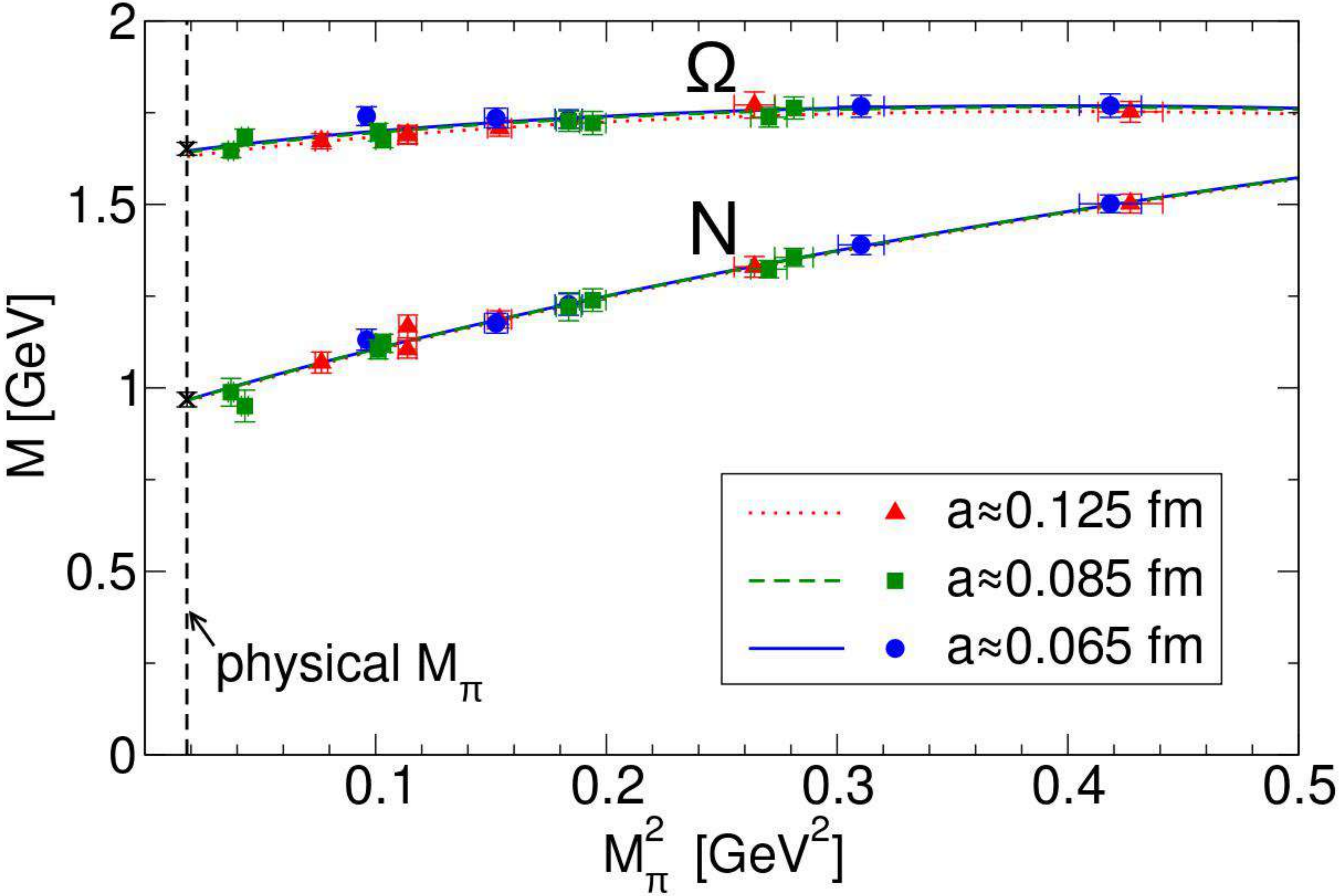
Autocorrelation time (finest lattice, small mass)

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

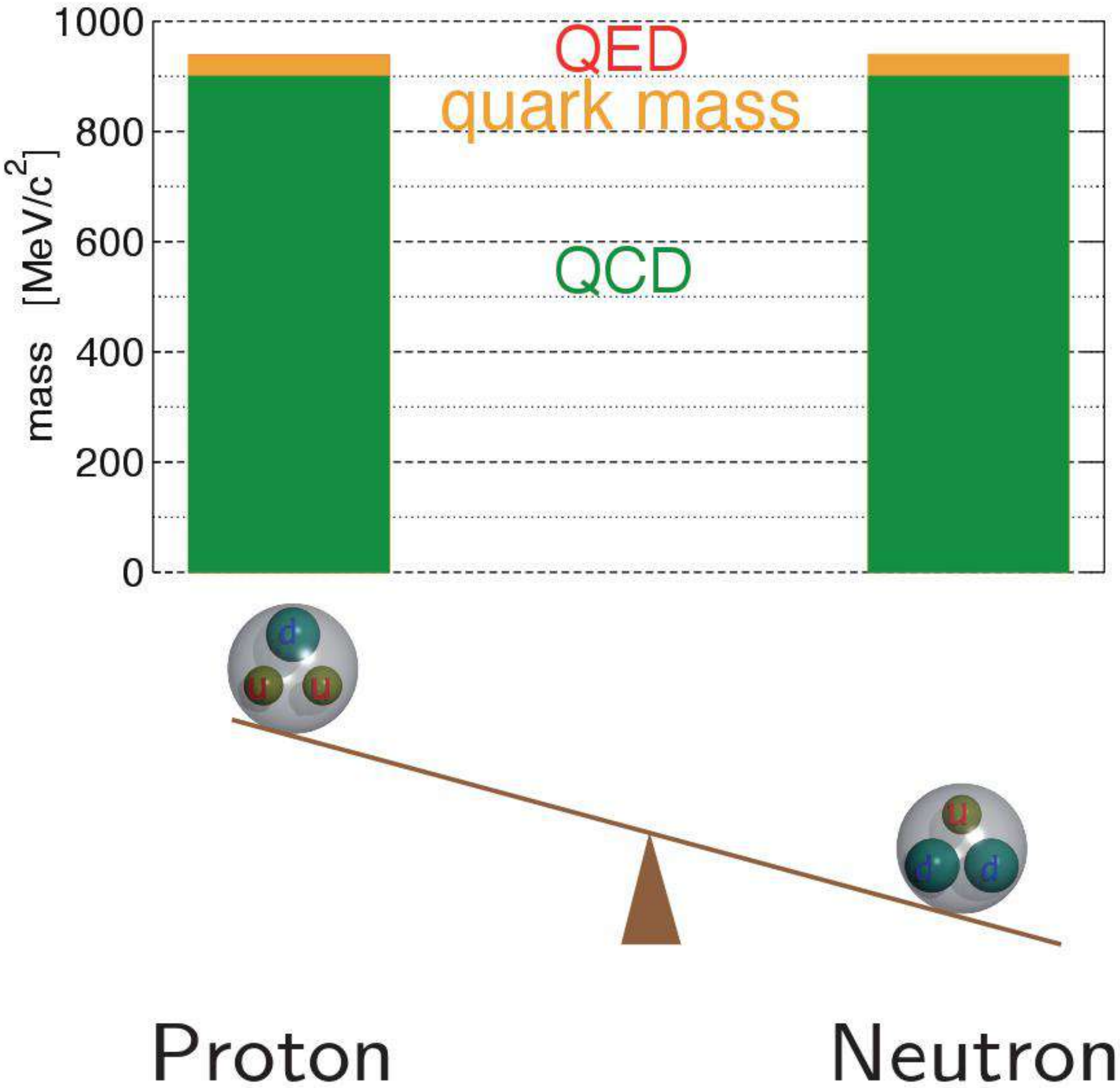
(MATLAB code from Wolff, 2004-7)



Chiral continuum fit



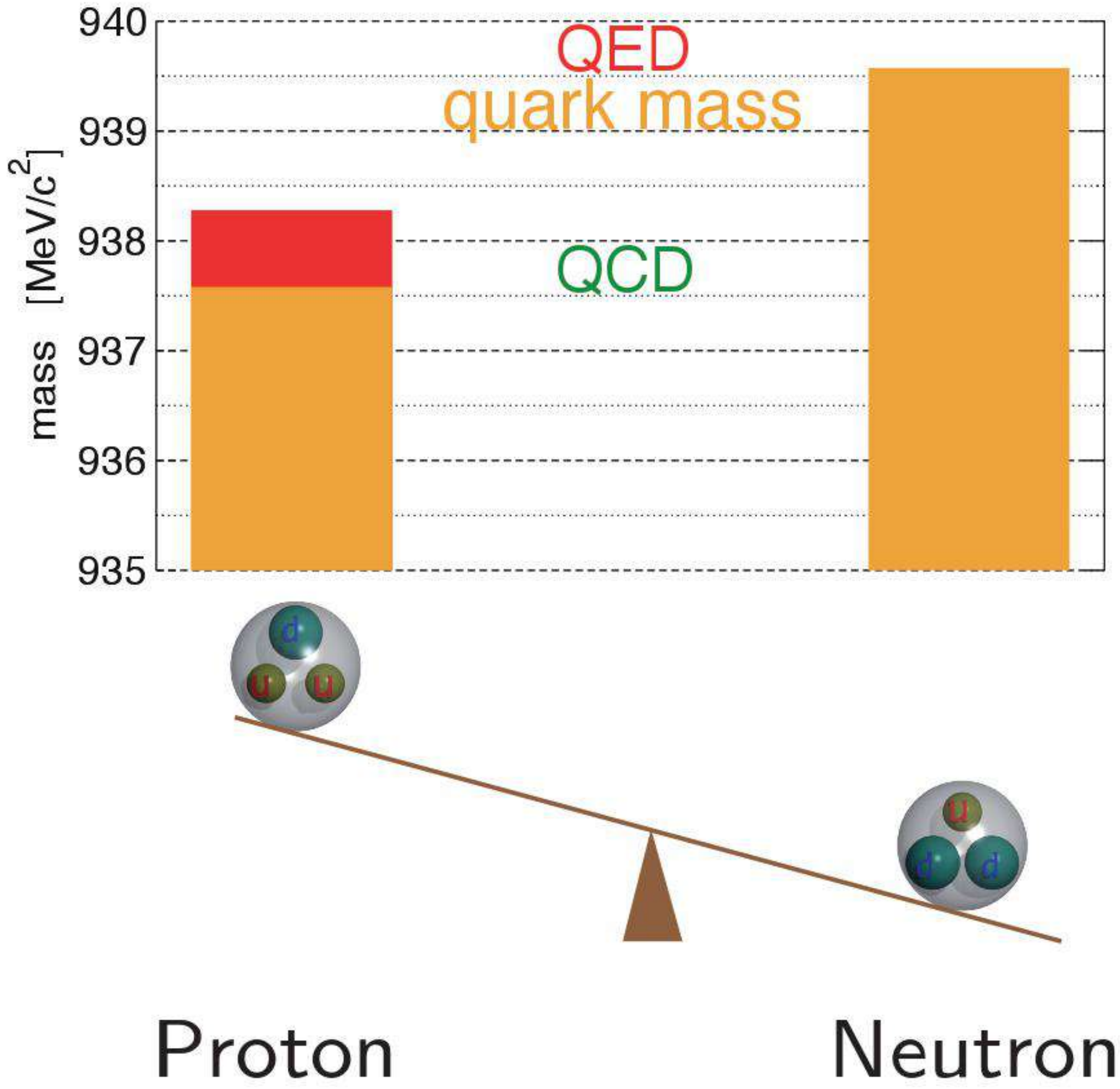
Is the fine structure relavant?



- Proton, neutron: 3 quarks
- Proton: uud
- Neutron: udd

- $m_u < m_d : M_p < M_n$
- $m_u = m_d : M_p > M_n$ Proton decays
- $M_p + M_{e^-} \gtrsim M_n$ No hydrogen

Is the fine structure relavant?



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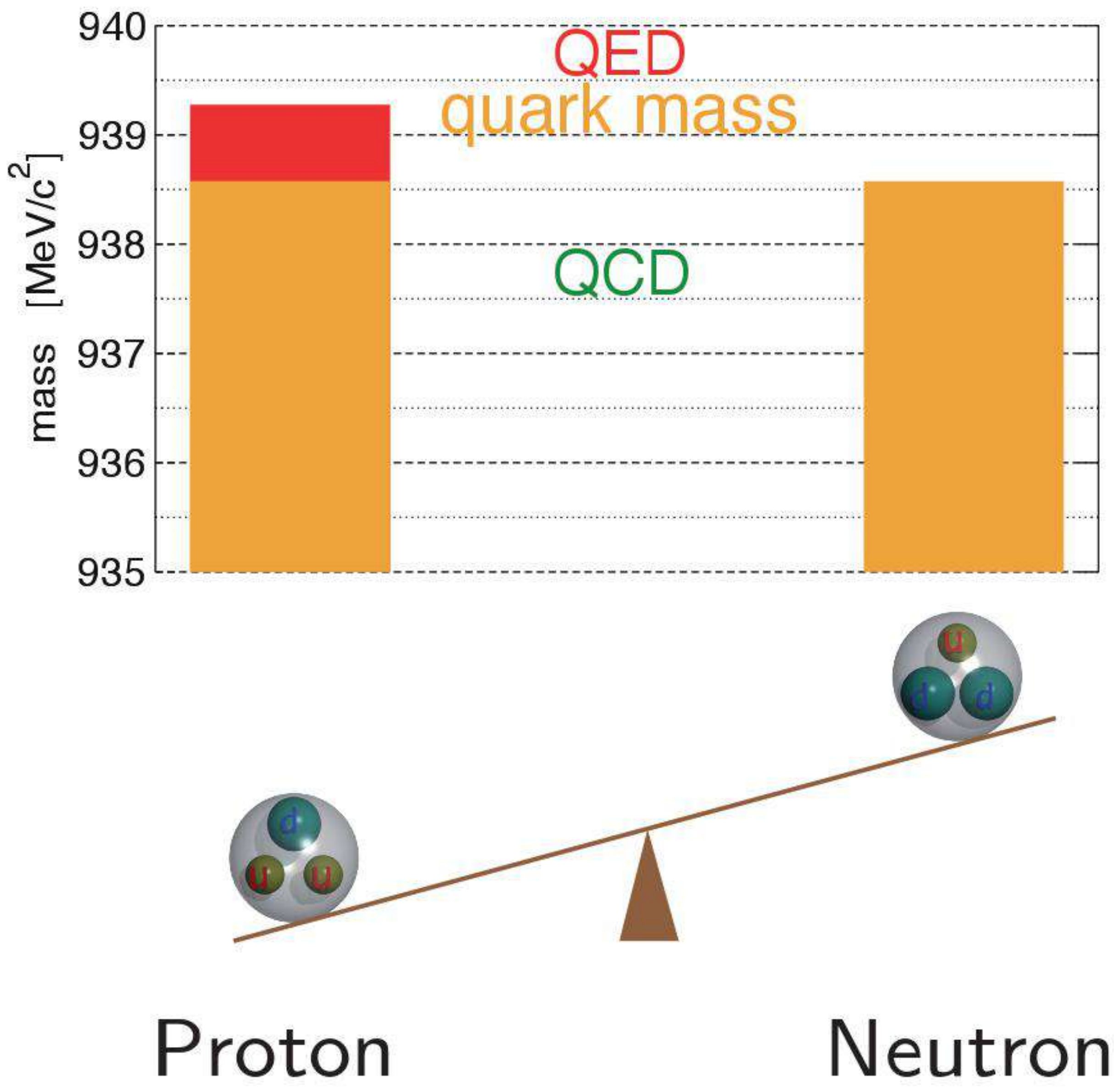

- Proton, neutron: 3 quarks
- Proton: uud
- Neutron: udd

- $m_u < m_d : M_p < M_n$
- $m_u = m_d : M_p > M_n$
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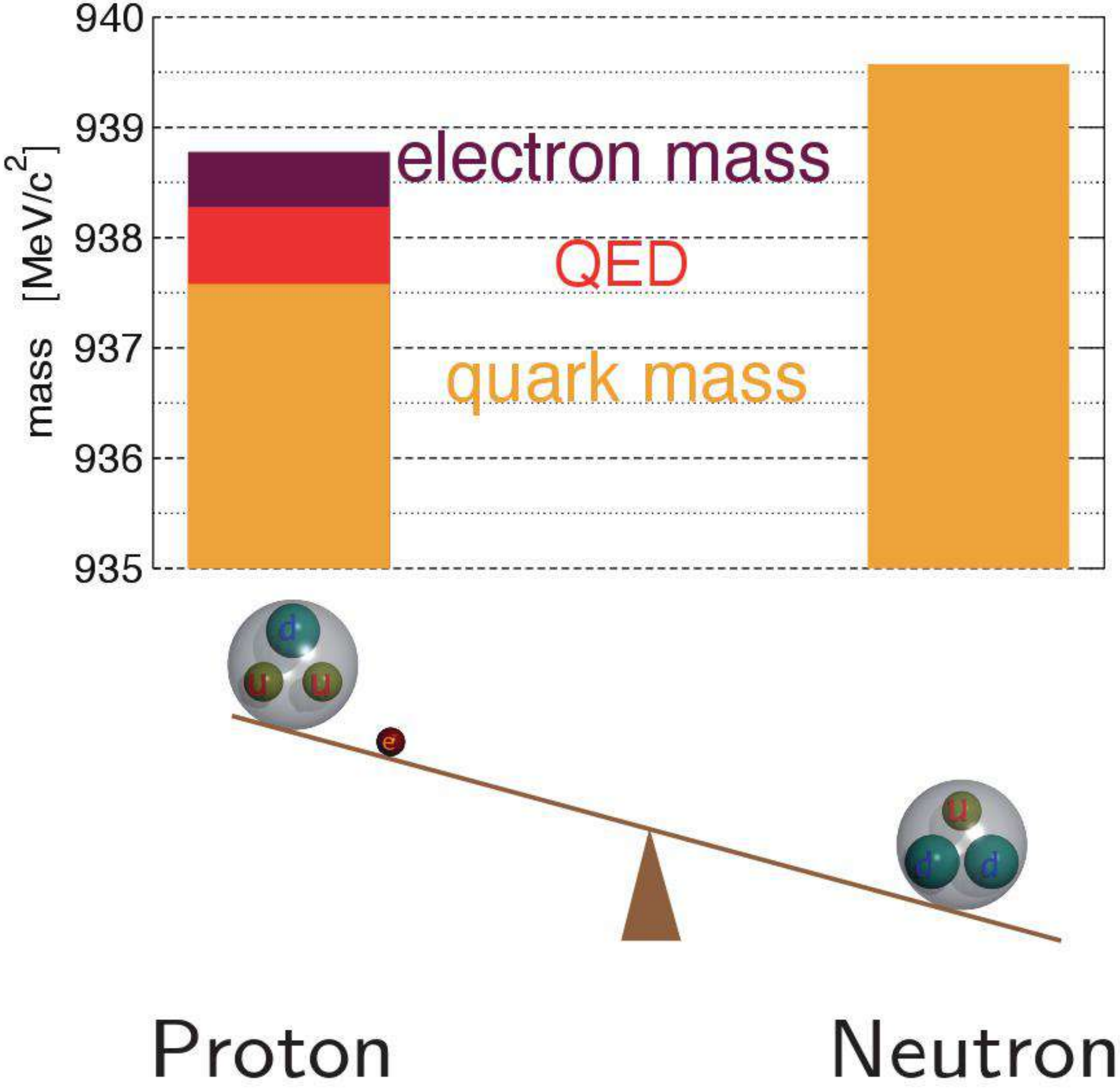
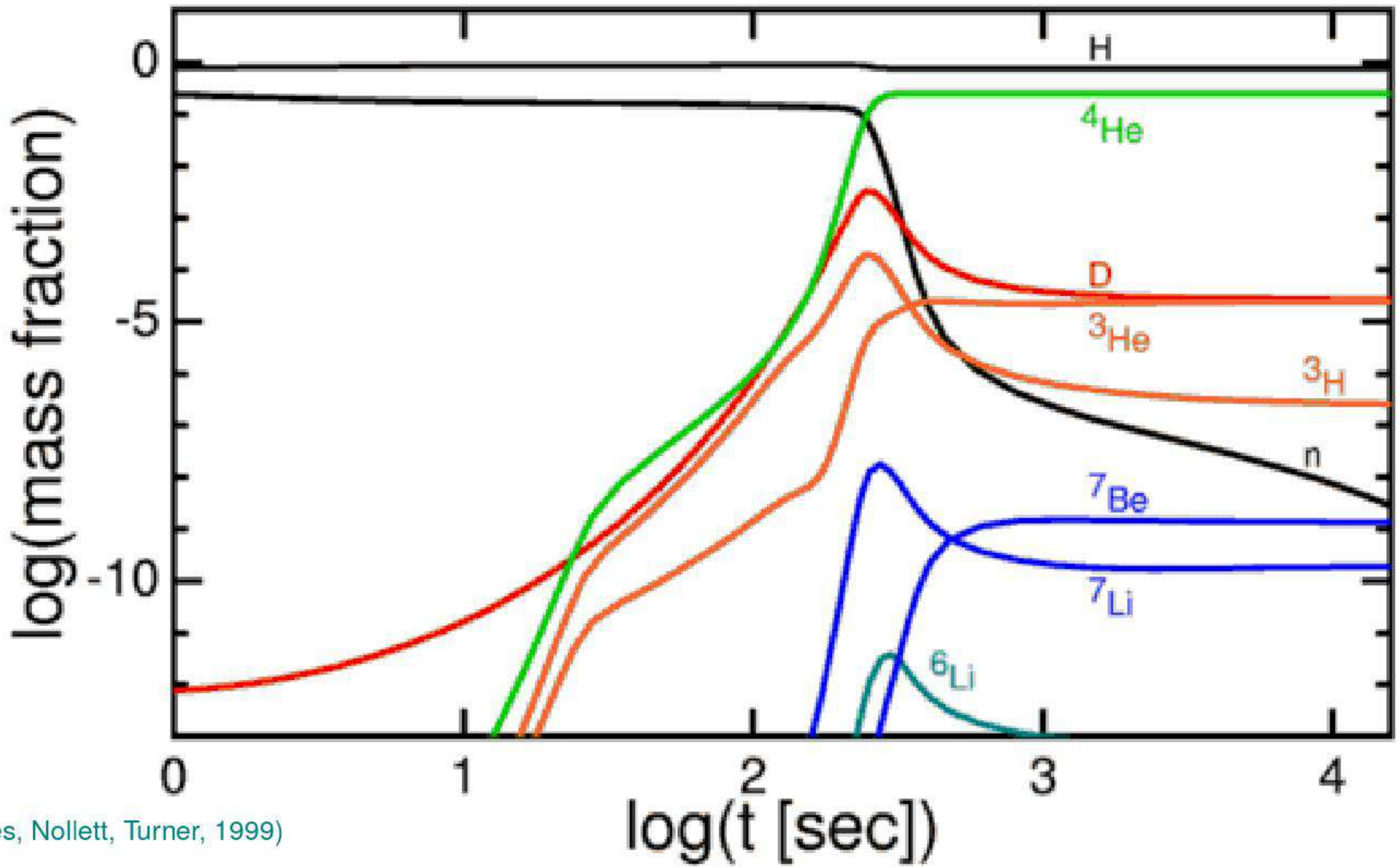


- Proton, neutron: 3 quarks
- Proton: uud
- Neutron: udd
- $m_u < m_d$: $M_p < M_n$
- $m_u = m_d$: $M_p > M_n$ Proton decays
- $M_p + M_{e^-} \gtrsim M_n$ No hydrogen

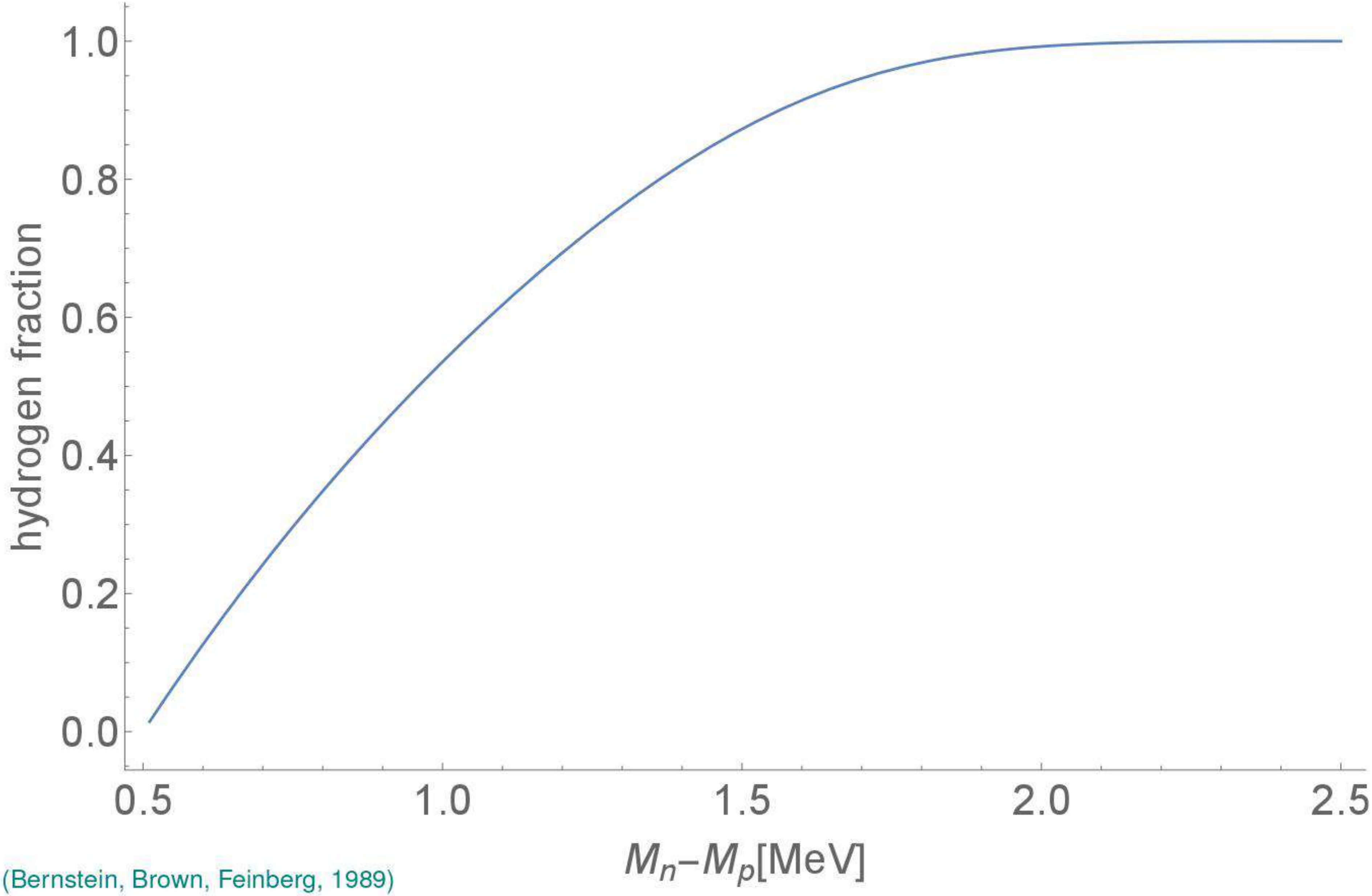
Big bang nucleosynthesis



(Burles, Nollett, Turner, 1999)

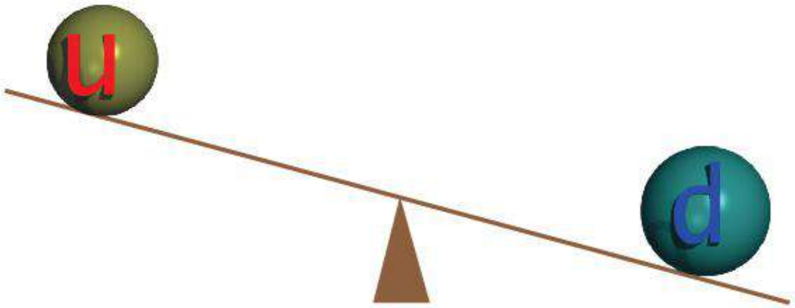
$M_n - M_p$ determines deuterium bottleneck

Hydrogen abundance



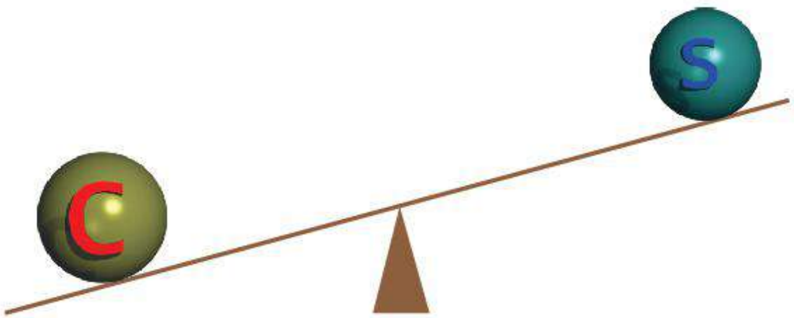
(Bernstein, Brown, Feinberg, 1989)

The light up quark

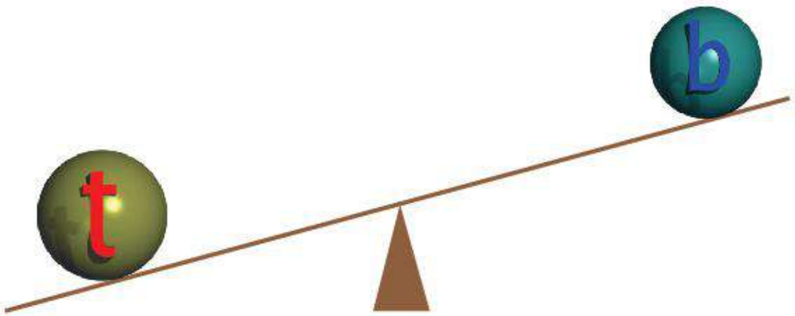


1st generation: $m_u < m_d$

Why?

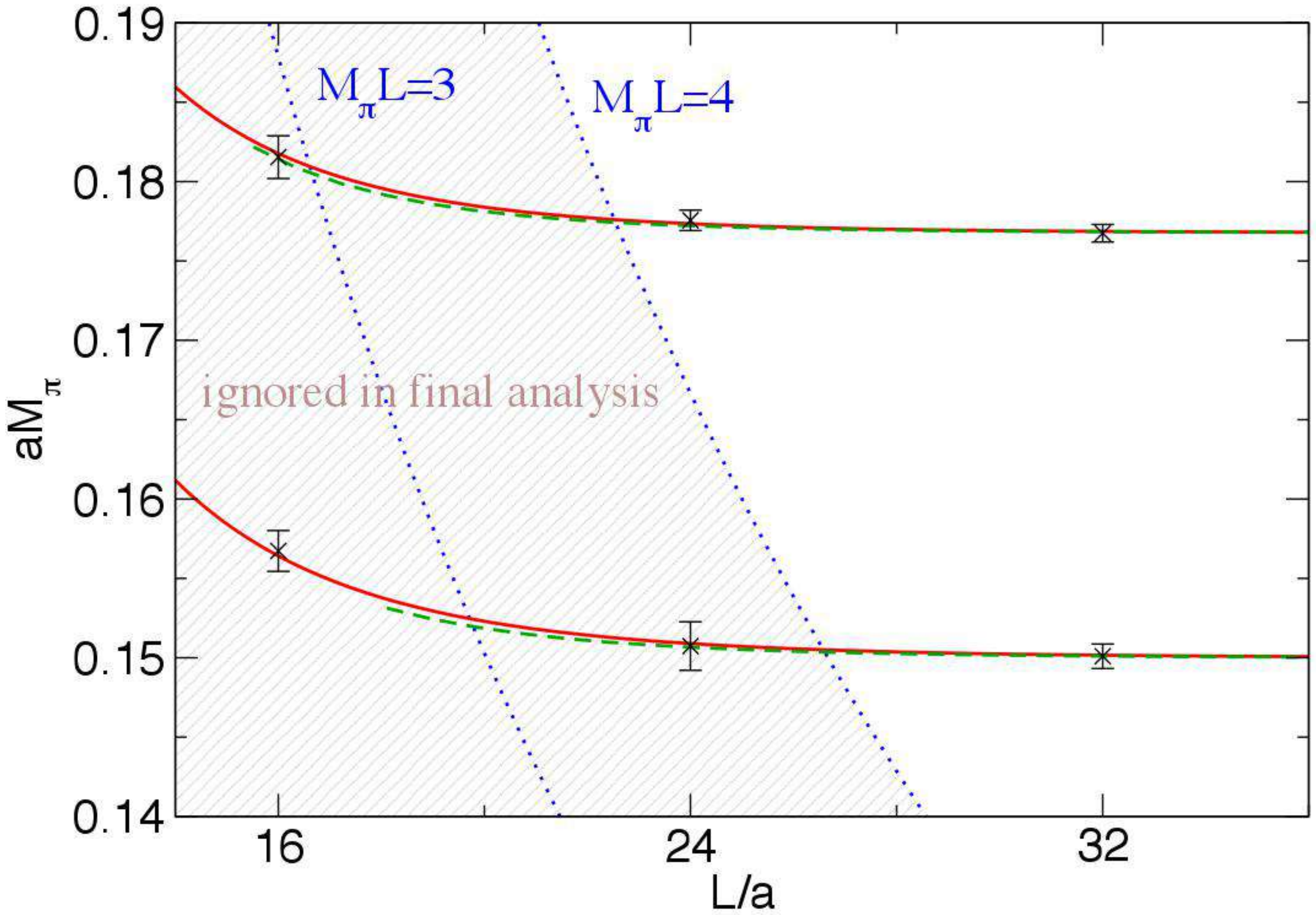


2nd generation: $m_c > m_s$



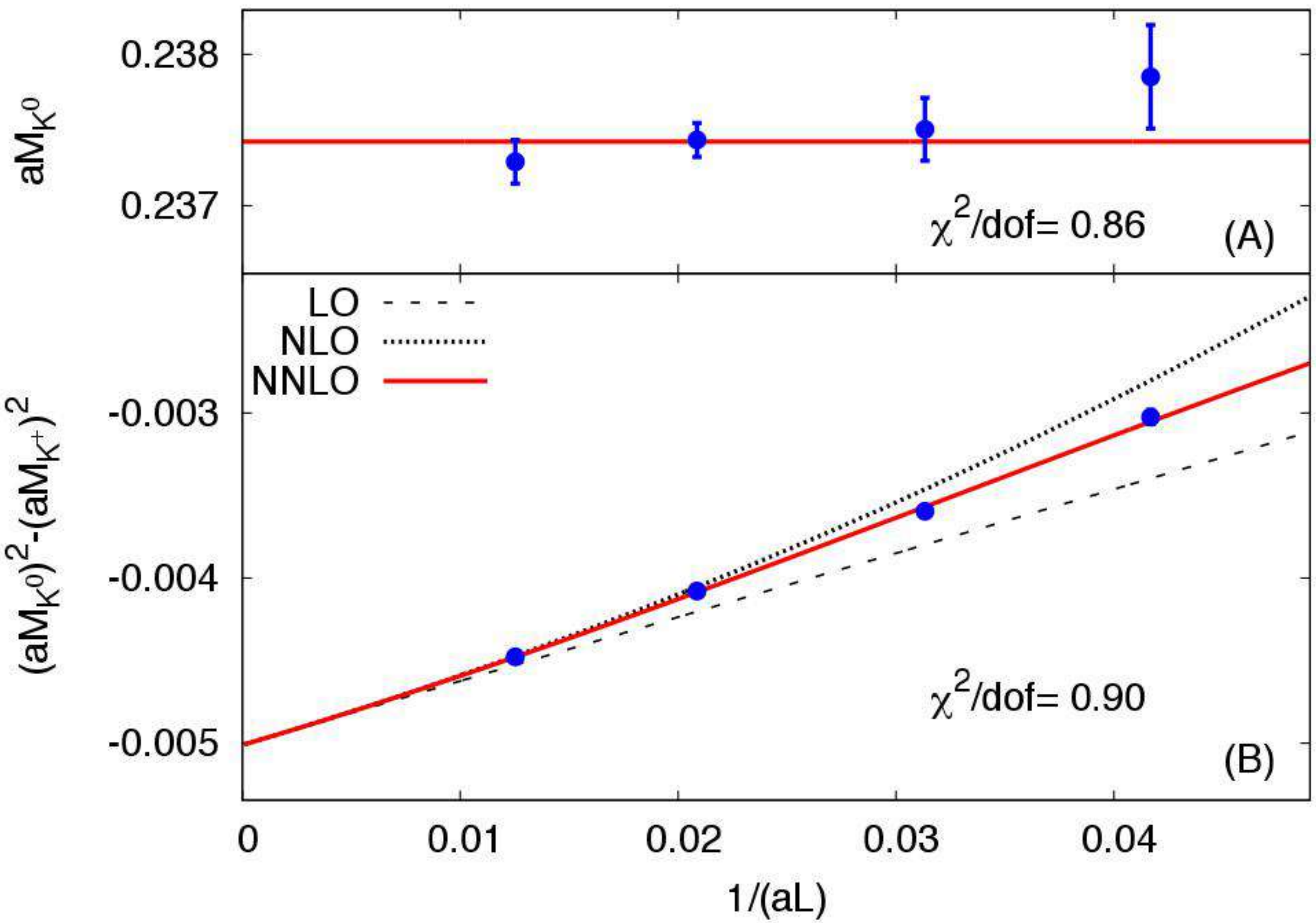
3rd generation: $m_t > m_b$

Tiny finite volume effects



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

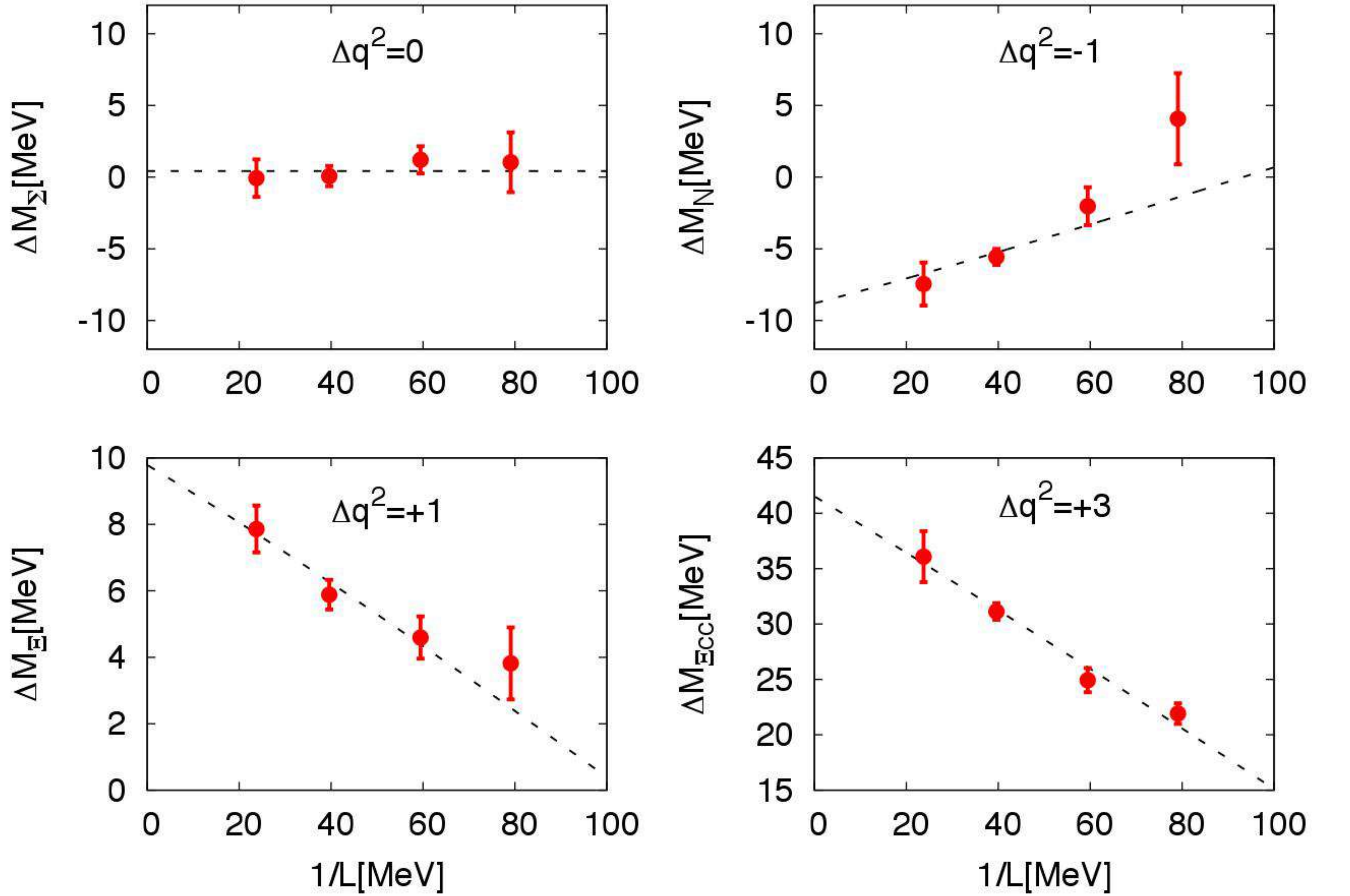
Universal FV effects



$$\delta m = q^2\alpha\left(\frac{\kappa}{2mL}\left(1+\frac{2}{mL}-\frac{3\pi}{(mL)^3}\right)\right)$$

(BMWc, 2014)

Baryon FV in QCD+QED



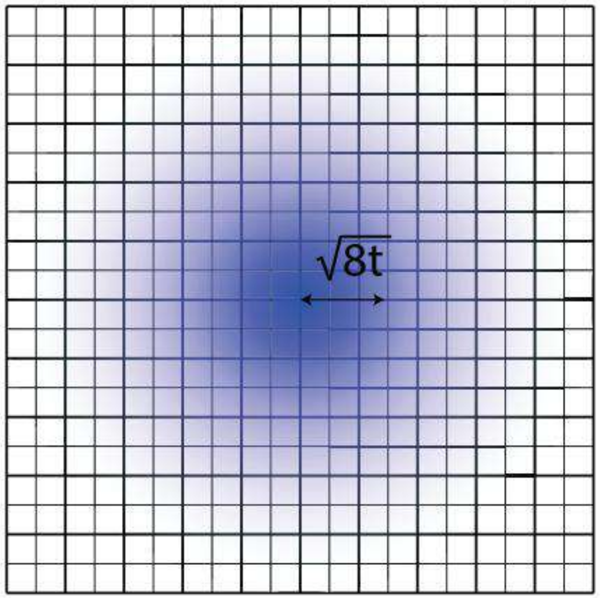
Identifying the physical point

We need to fix 6 parameters: m_u, m_d, m_s, m_c,, α_s and α

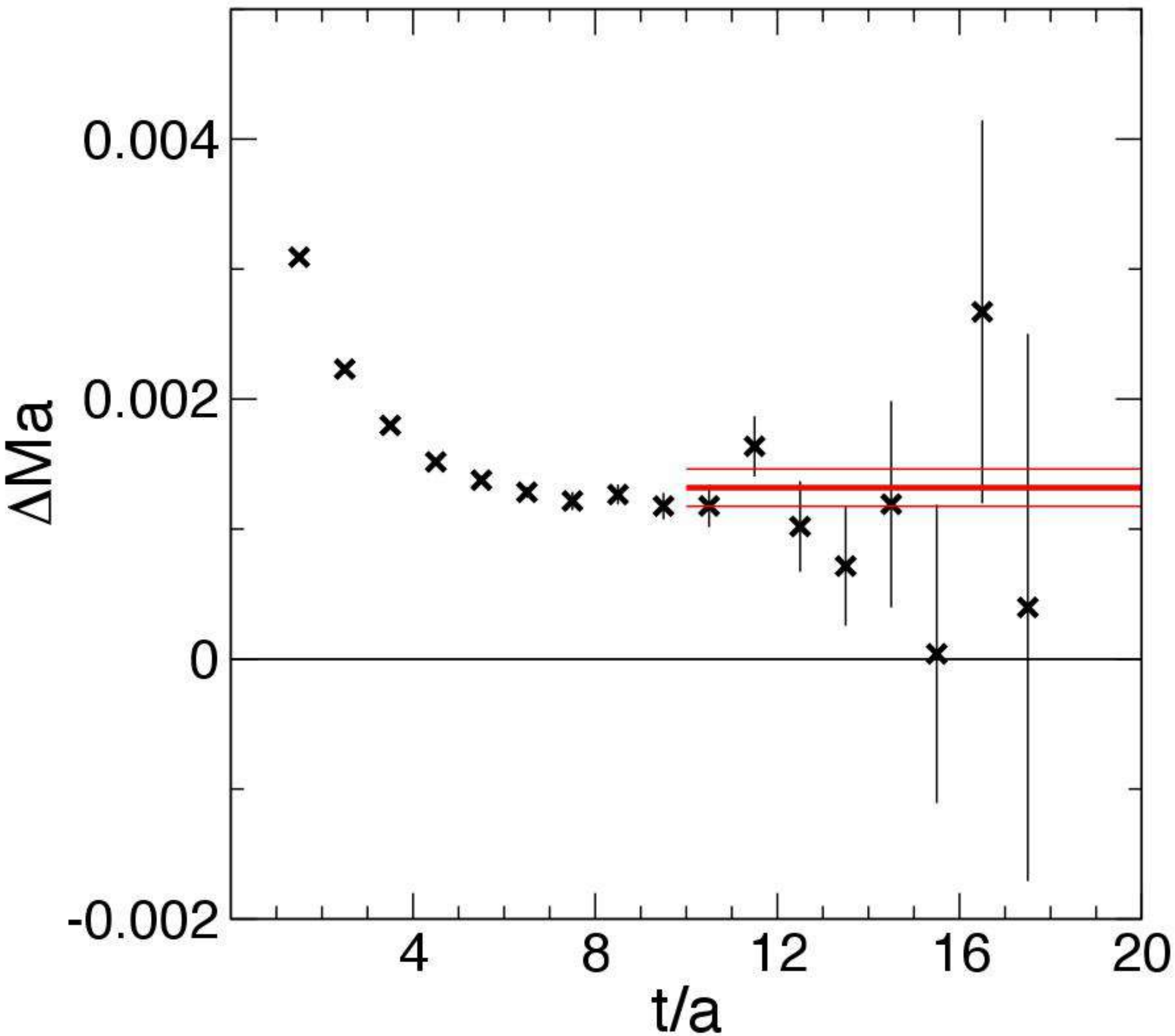
- Requires fixing 5 dimensionless ratios from 6 lattice observables
- 4 "canonical" lattice observables: $M_{\pi^\pm}$, M_{K^+}, M_Ω, M_D
- Strong isospin splitting from $M_{K^\pm} - M_{K^0}$
- what about α?
  - ✗ From $M_{\pi^\pm} - M_{\pi^0}$ ➛ disconnected diagrams, very noisy
  - ✗ From e^- e^- scattering ➛ far too low energy
  - ✗ From $M_{\Sigma^+} - M_{\Sigma^-}$ ➛ baryon has inferior precision
  - ✓ Take renormalized α as input directly
  - ➛ Use the QED gradient flow
    Analytic tree level correction

$$\langle F_{\mu\nu} F_{\mu\nu} \rangle = \frac{6}{V_4} \sum_k e^{-2|\hat{k}|^2 t}$$

Slightly more complicated for clover plaquette



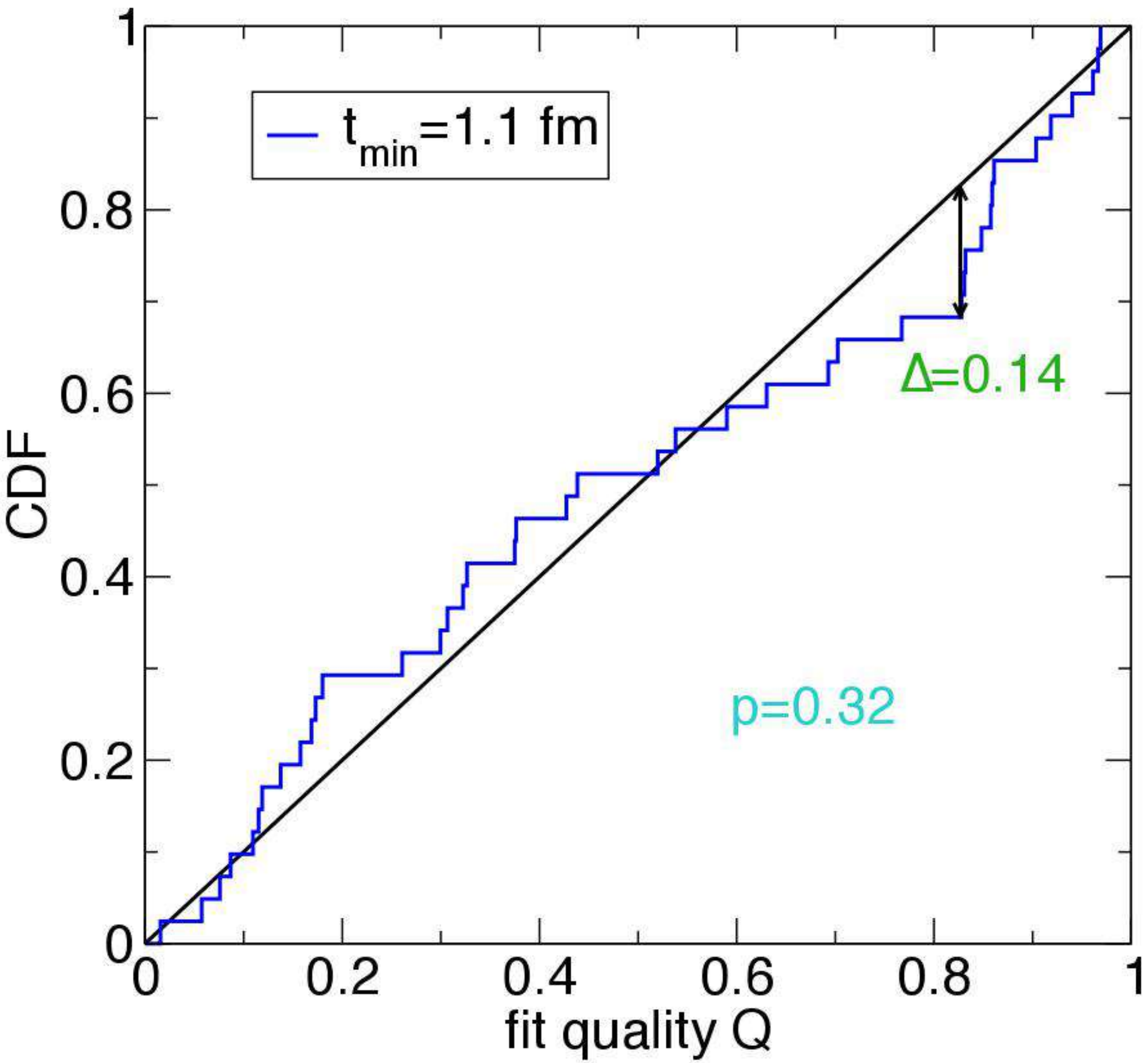
Plateaux



- Fit range is critical
- Exclude excited states
- Determine from data

Conservative method:
Check that fit quality is a flat random distribution in $(0, 1)$

Plateaux range



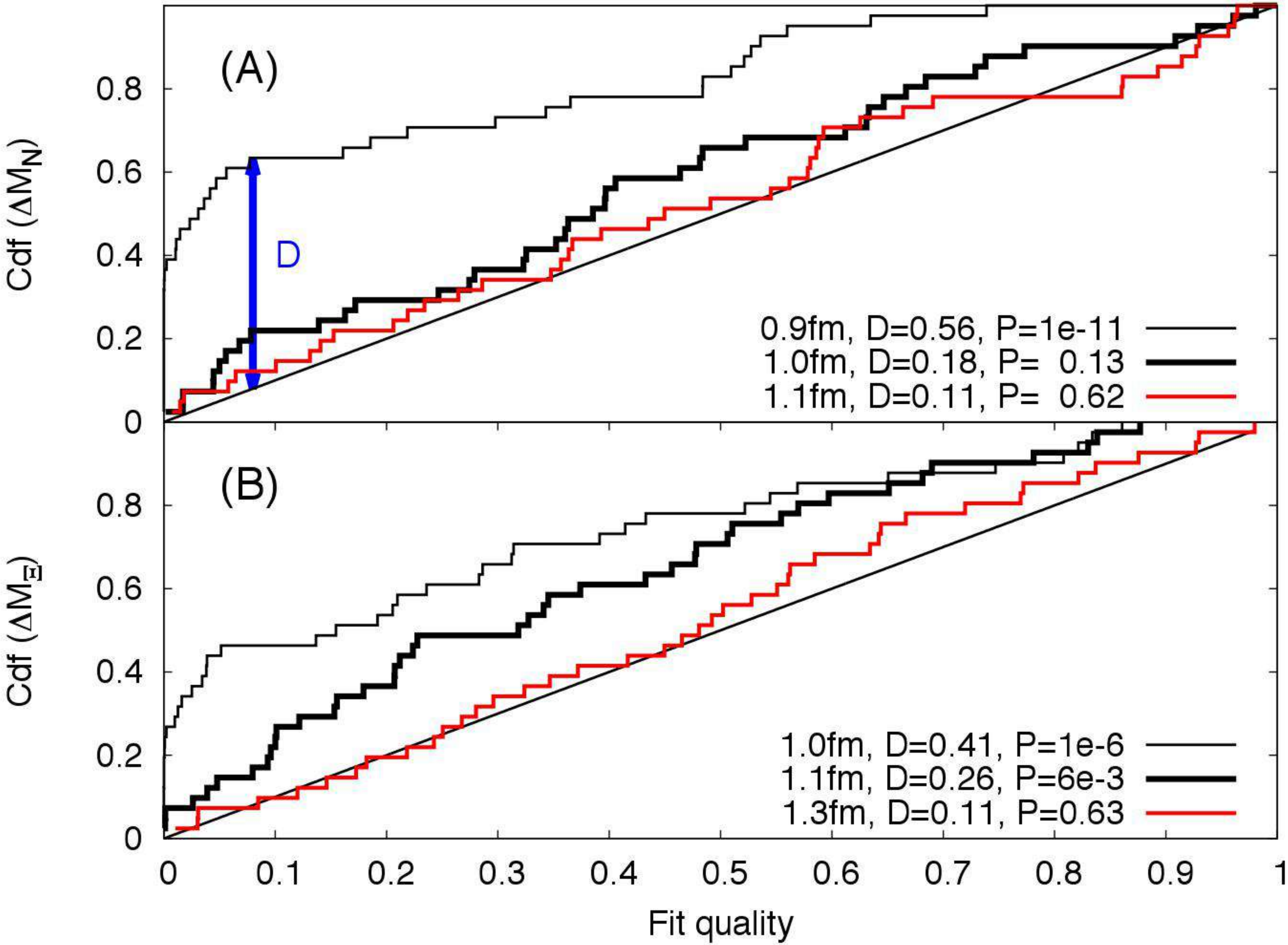
- Need many ensembles
- Plot CDF
- KS test flat distribution

$P(\Delta > \text{observed})$:

$$p\left(\Delta\left(\sqrt{N} + 0.12 + \frac{0.11}{\sqrt{N}}\right)\right)$$

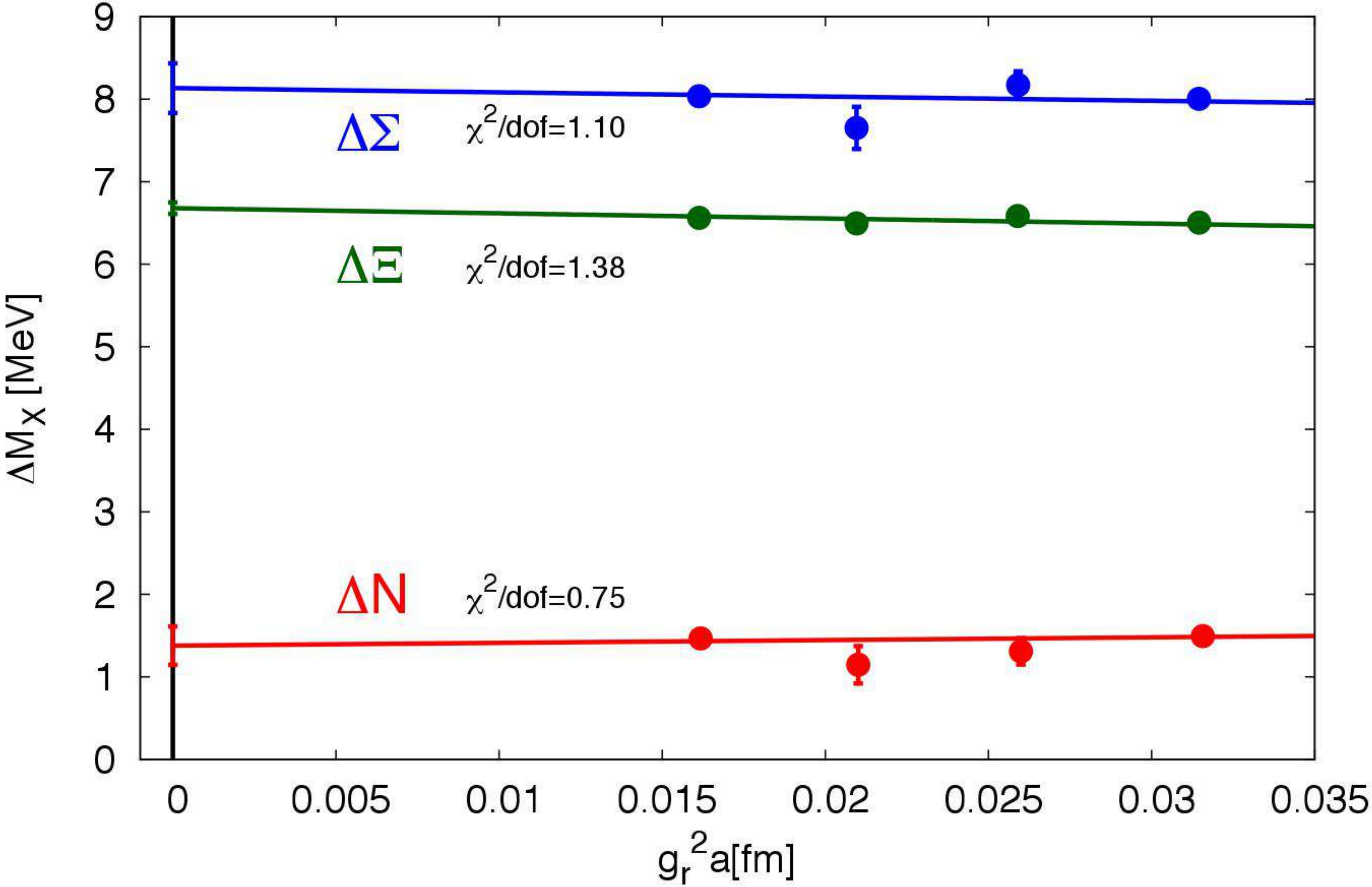
with

$$p(x) = \sum_j \frac{(-)^{j-1}2}{e^{-2j^2x^3}}$$



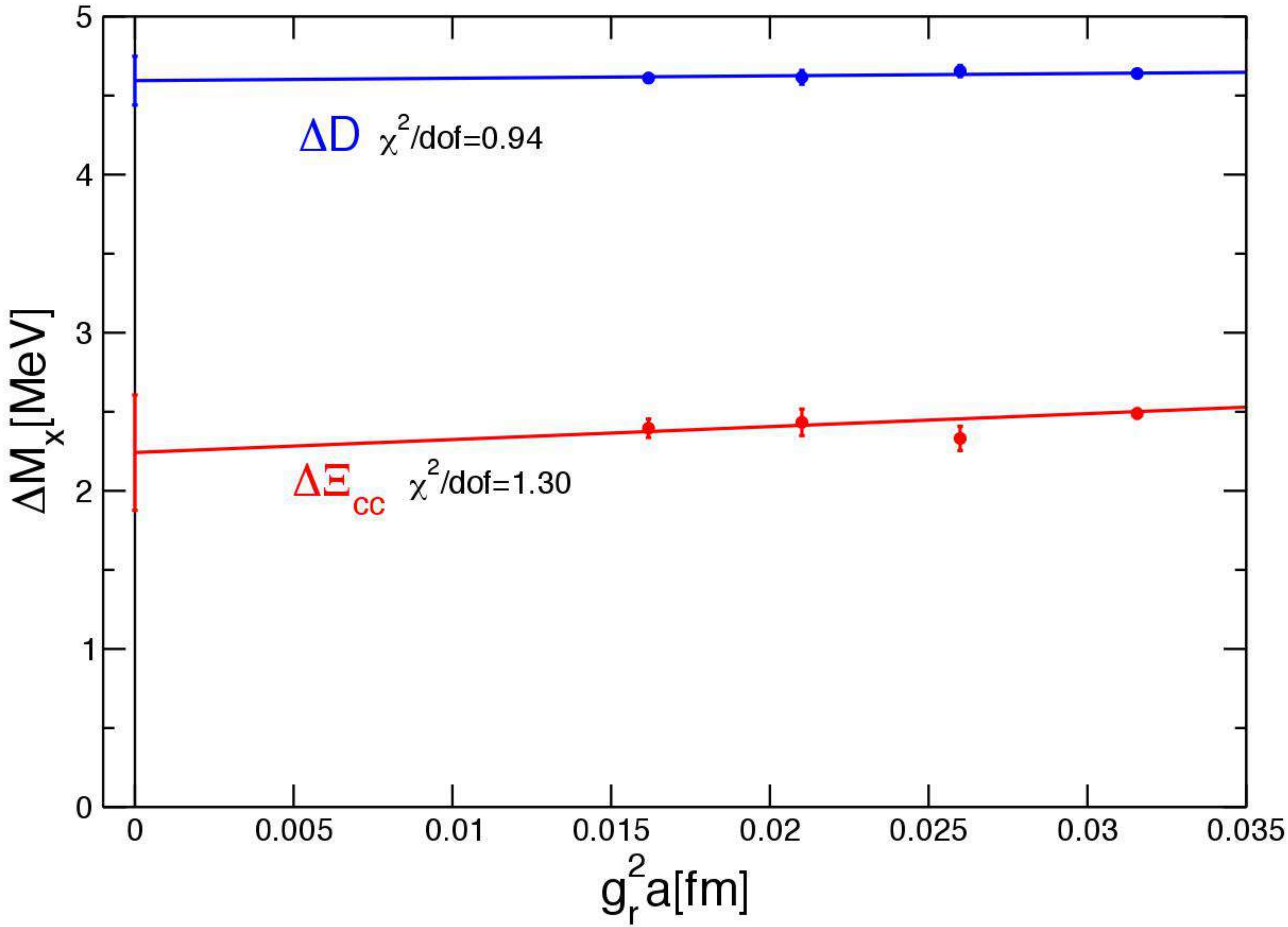
(A)
Cdf (ΔM_N)
D
0.9fm, D=0.56, P=1e-11
1.0fm, D=0.18, P= 0.13
1.1fm, D=0.11, P= 0.62
(B)
Cdf (ΔM_Ξ)
1.0fm, D=0.41, P=1e-6
1.1fm, D=0.26, P=6e-3
1.3fm, D=0.11, P=0.63
Fit quality
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
0 0.2 0.4 0.6 0.8

Scaling



9
8
7
6
5
4
3
2
1
0
ΔΣ
χ²/dof=1.10
ΔΞ
χ²/dof=1.38
ΔN
χ²/dof=0.75
ΔM_X [MeV]
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
g_r²a[fm]

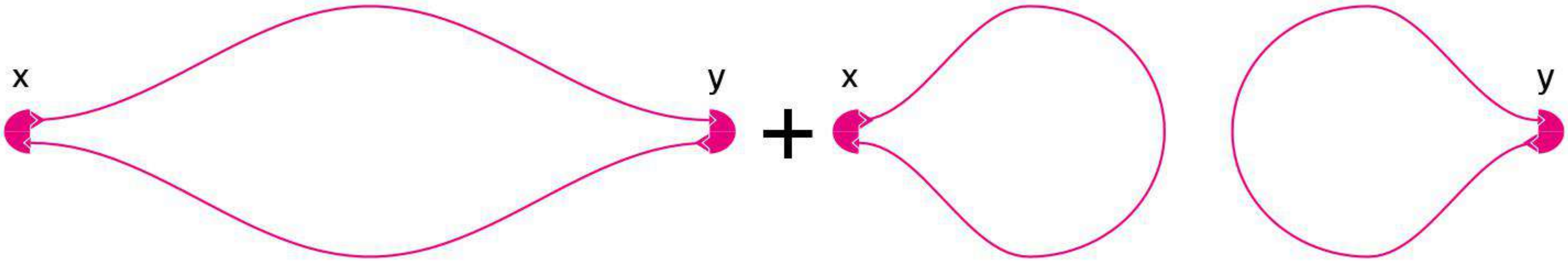
Scaling


ΔD χ²/dof=0.94
ΔΞcc χ²/dof=1.30
ΔMx[MeV]
g_r² a[fm]
0
1
2
3
4
5
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035

Disentangling contributions

Problem:

- Disentangle QCD and QED contributions
  - Not unique, $O(\alpha^2)$ ambiguities
- Flavor singlet (e.g. π^0) difficult (disconnected diagrams)



Method:

- Use baryonic splitting Σ^+-Σ^- purely QCD
  - Only physical particles
  - Exactly correct for pointlike particle
  - Corrections below the statistical error

Isospin splittings numerical values

	splitting [MeV]	QCD [MeV]	QED [MeV]
$\Delta N = n - p$	1.51(16)(23)	2.52(17)(24)	-1.00(07)(14)
$\Delta\Sigma = \Sigma^- - \Sigma^+$	8.09(16)(11)	8.09(16)(11)	0
$\Delta\Xi = \Xi^- - \Xi^0$	6.66(11)(09)	5.53(17)(17)	1.14(16)(09)
$\Delta D = D^\pm - D^0$	4.68(10)(13)	2.54(08)(10)	2.14(11)(07)
$\Delta\Xi_{cc} = \Xi_{cc}^{++} - \Xi_{cc}^{+}$	2.16(11)(17)	-2.53(11)(06)	4.69(10)(17)
$\Delta_{CG} = \Delta N - \Delta\Sigma + \Delta\Xi$	0.00(11)(06)	-0.00(13)(05)	0.00(06)(02)

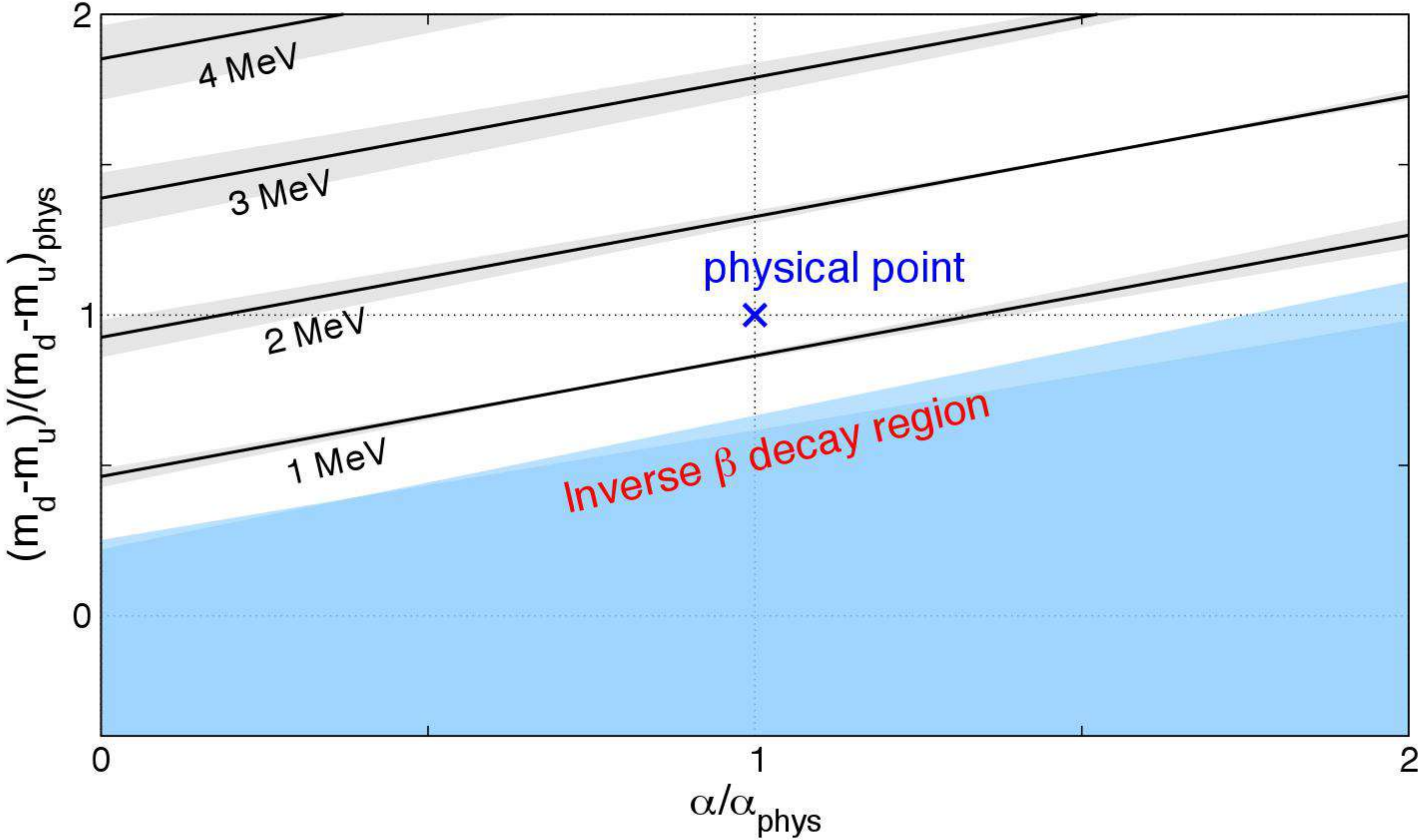
- Quark model relation predicts Δ_{CG} to be small

(Coleman, Glashow, 1961; Zweig 1964)

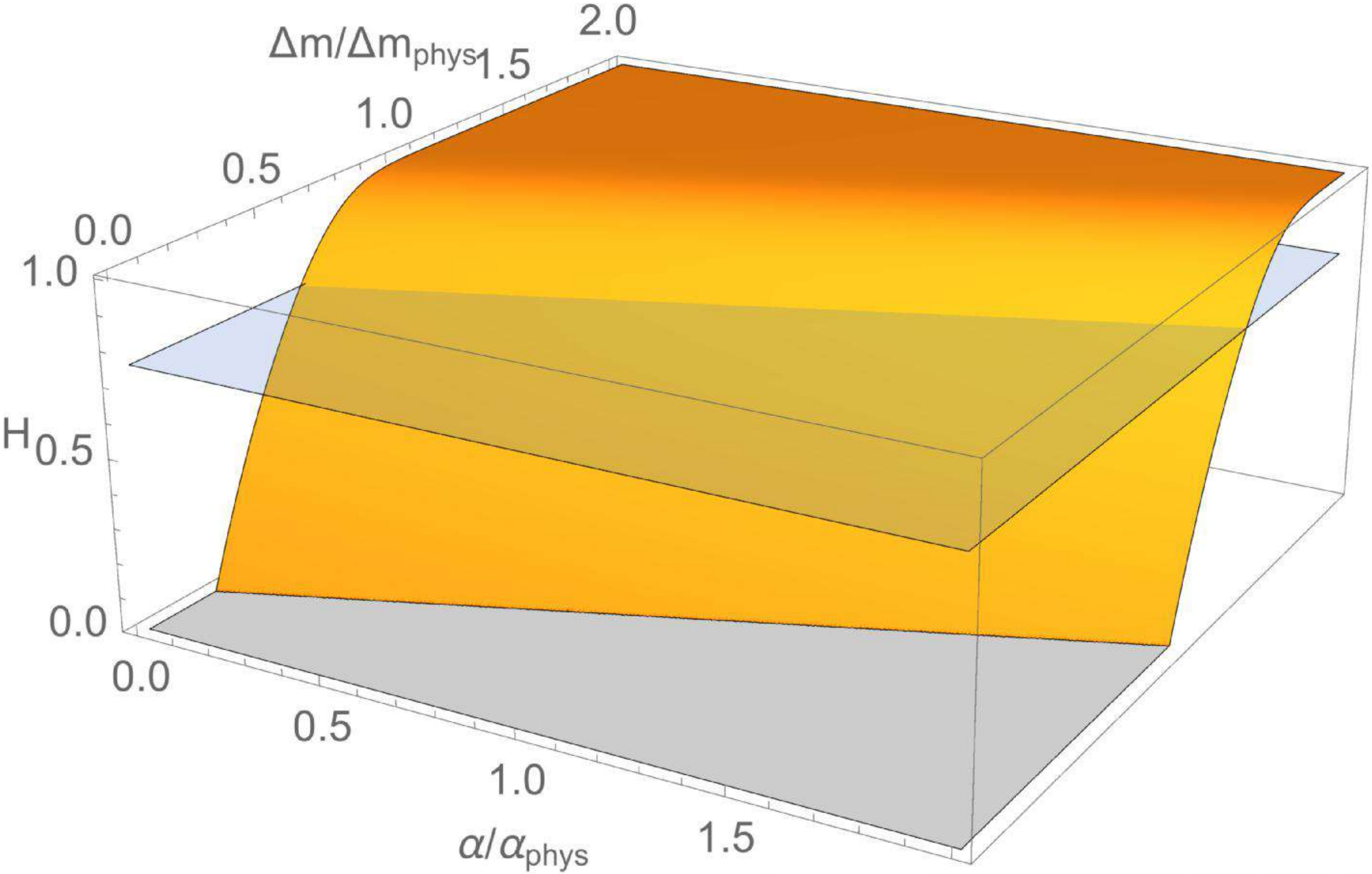
$$\Delta_{CG} = M(udd) + M(uus) + M(dss) - M(uud) - M(dds) - M(uss)$$

$$\Delta_{CG} \propto ((m_d - m_u)(m_s - m_u)(m_s - m_d), \alpha(m_s - m_d))$$

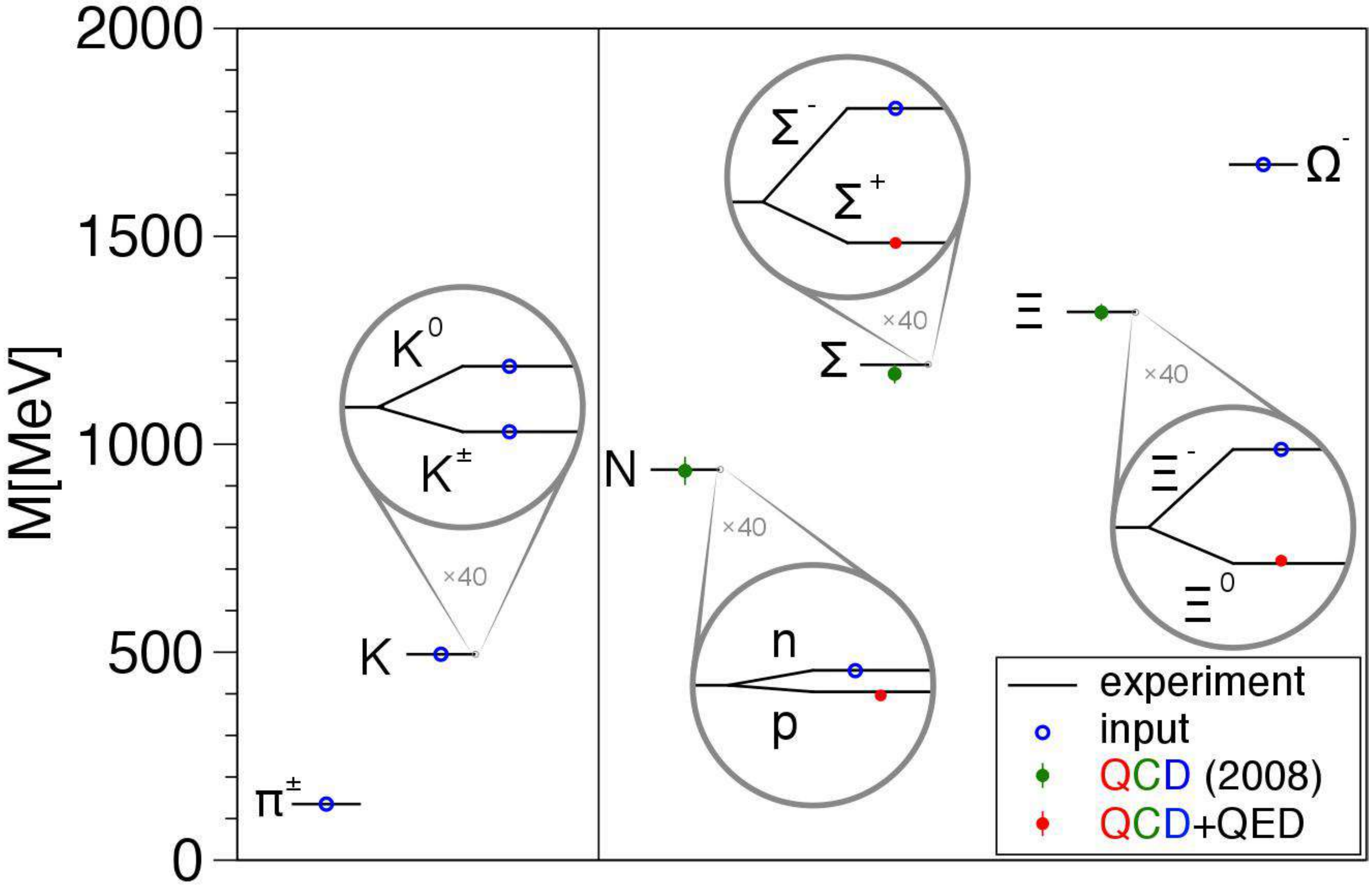
Nucleon splitting QCD and QED parts



Resulting initial hydrogen abundance

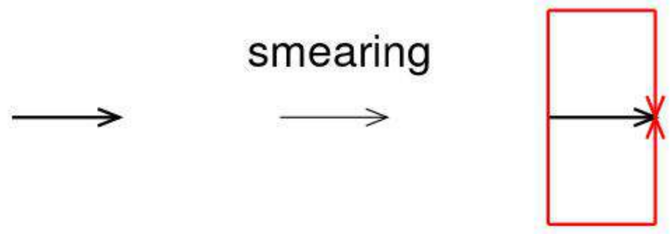


PROGRESS



2000
1500
1000
500
0
M[MeV]
π±
K
K0
K±
×40
N
n
p
Σ
Σ-
Σ+
Ξ
Ξ-
Ξ0
Ω-
experiment
input
QCD (2008)
QCD+QED

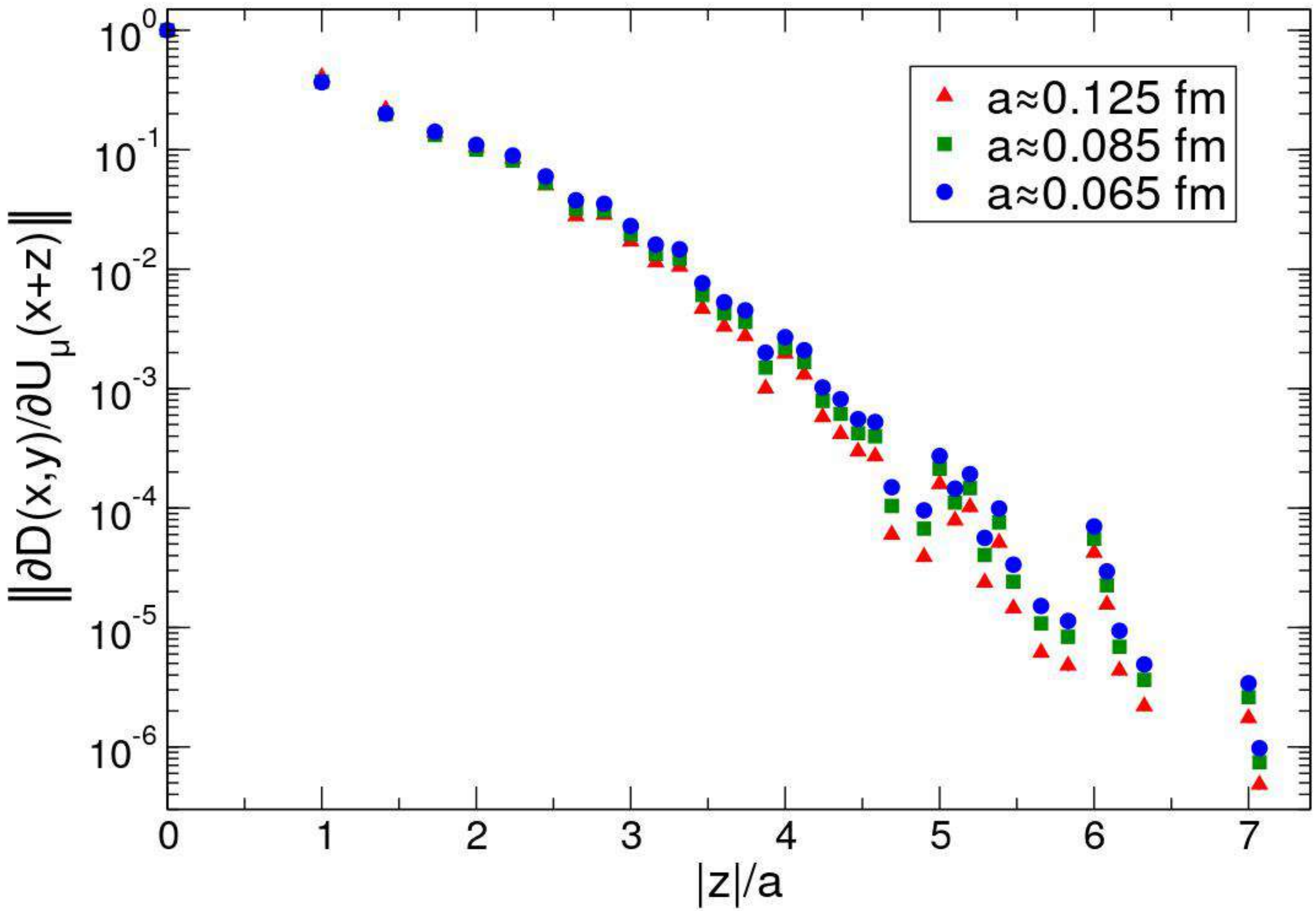
Locality properties



- 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:



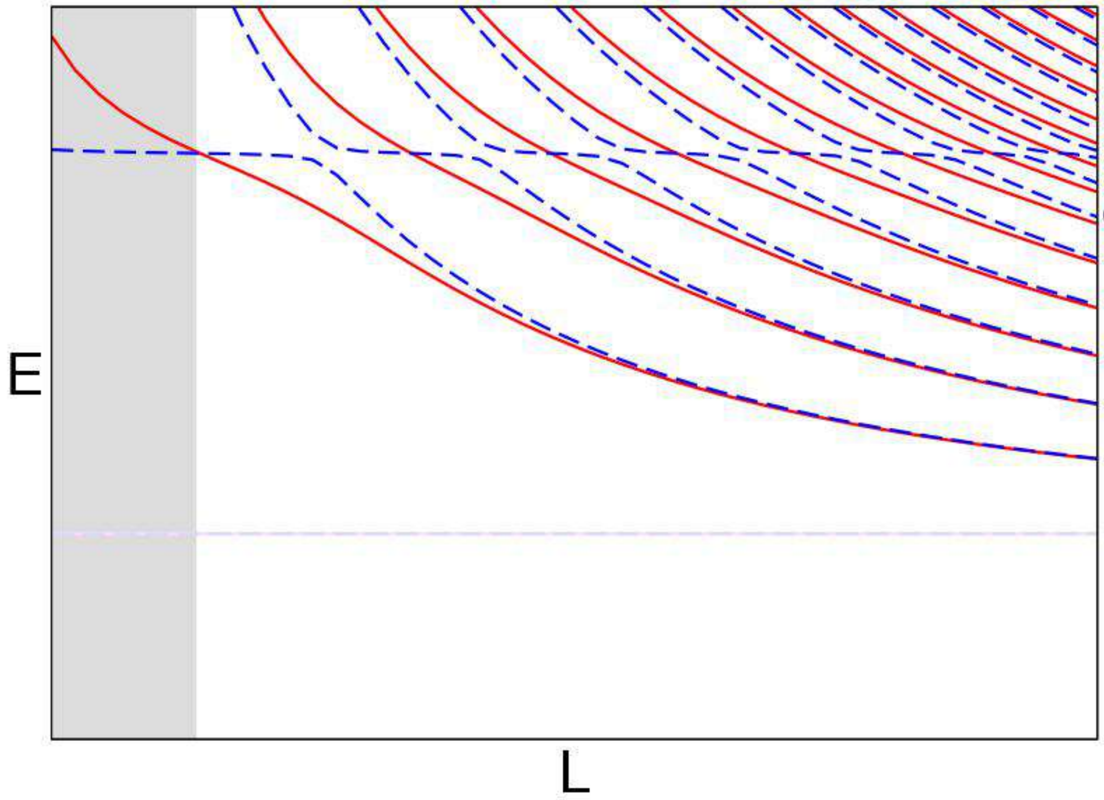
Finite volume effects in resonances

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

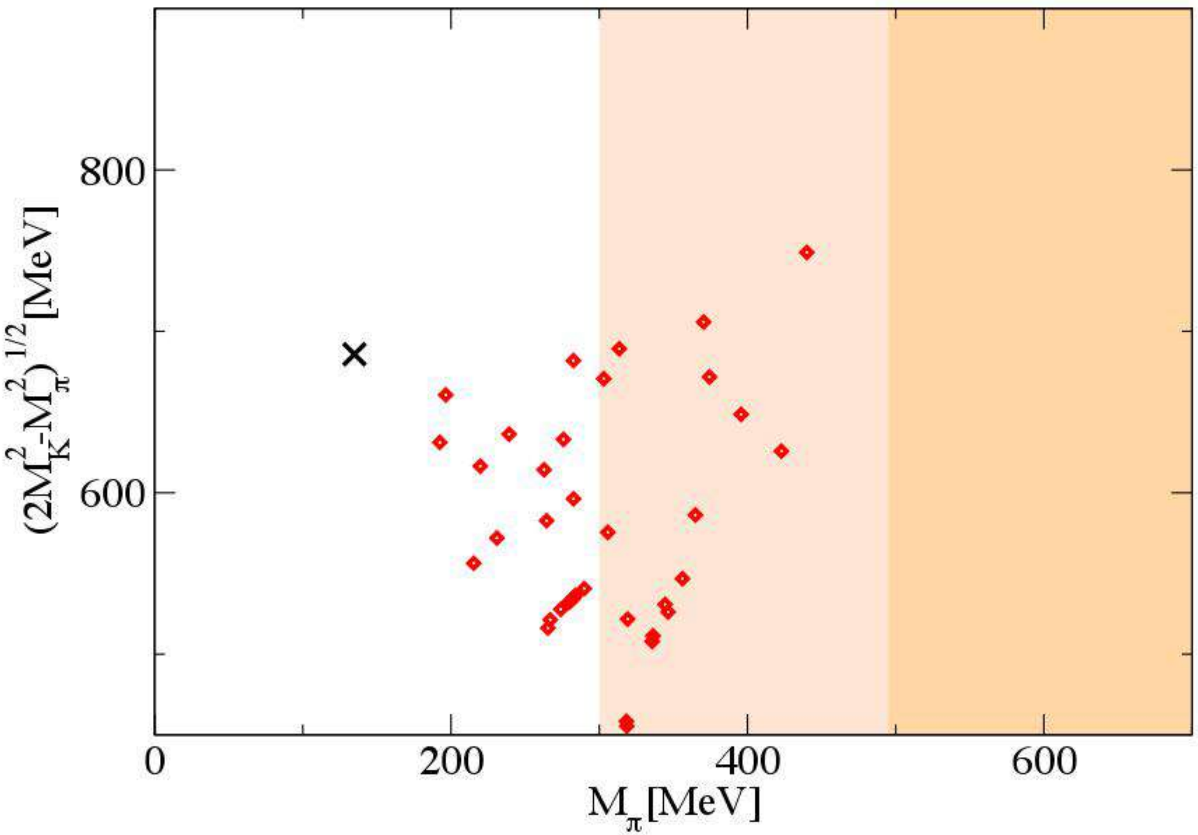


- Treatment as scattering problem

(Lüscher, 1985-1991)

  - Parameters: mass and coupling (width)
  - Alternative approaches suggested

Landscape



- Small extrapolation to physical point
- Charm mass is physical
- $u - d$ splitting is physical
- Why use $\alpha \gg \alpha^{\text{phys}}$?

- Hadron masses are even in e, so signal $\propto e^2$
- Per configuration fluctuations are not even in e, so noise $\propto e$
- Per configuration cancellation helps in qQED, but not dynamically

Systematic uncertainties

Goal:

- Accurately estimate total systematic error

Method:

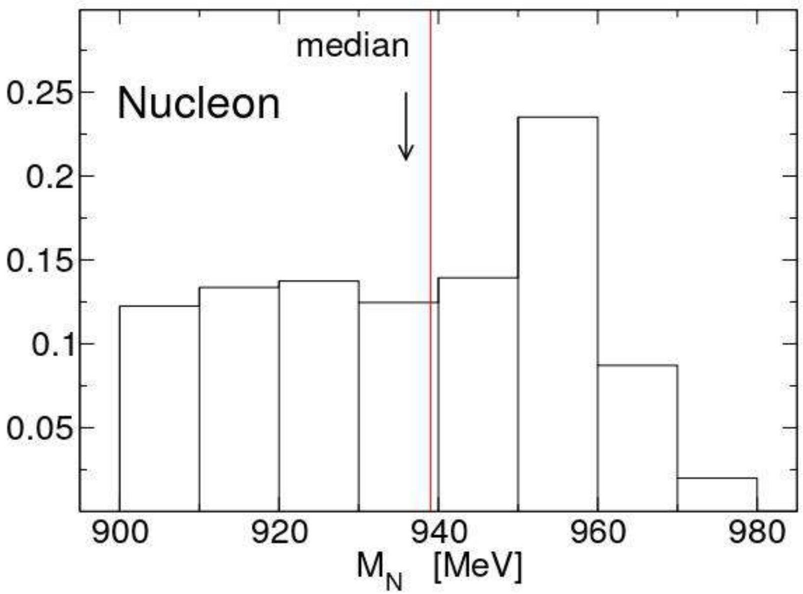
- We account for all the above mentioned effects
- When there are a number of sensible ways to proceed, we take them: Complete analysis for each of
  - 18 fit range combinations
  - ratio/nonratio fits (r_X resp. M_X)
  - $O(a)$ and $O(a^2)$ discretization terms
  - NLO χPT M_π^3 and Taylor M_π^4 chiral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

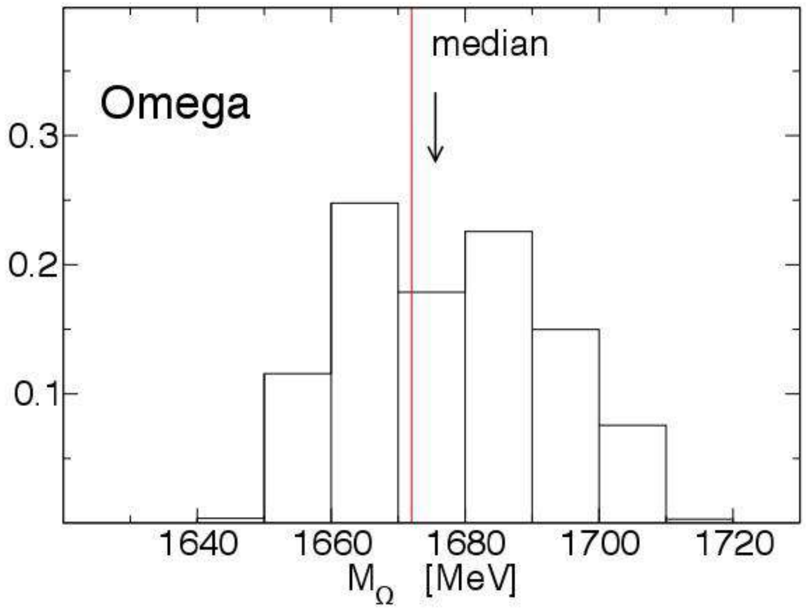
  resulting in 432 (144) predictions for each baryon (vector meson) mass with each 2000 bootstrap samples for each Ξ and Ω scale setting

Systematic uncertainties II

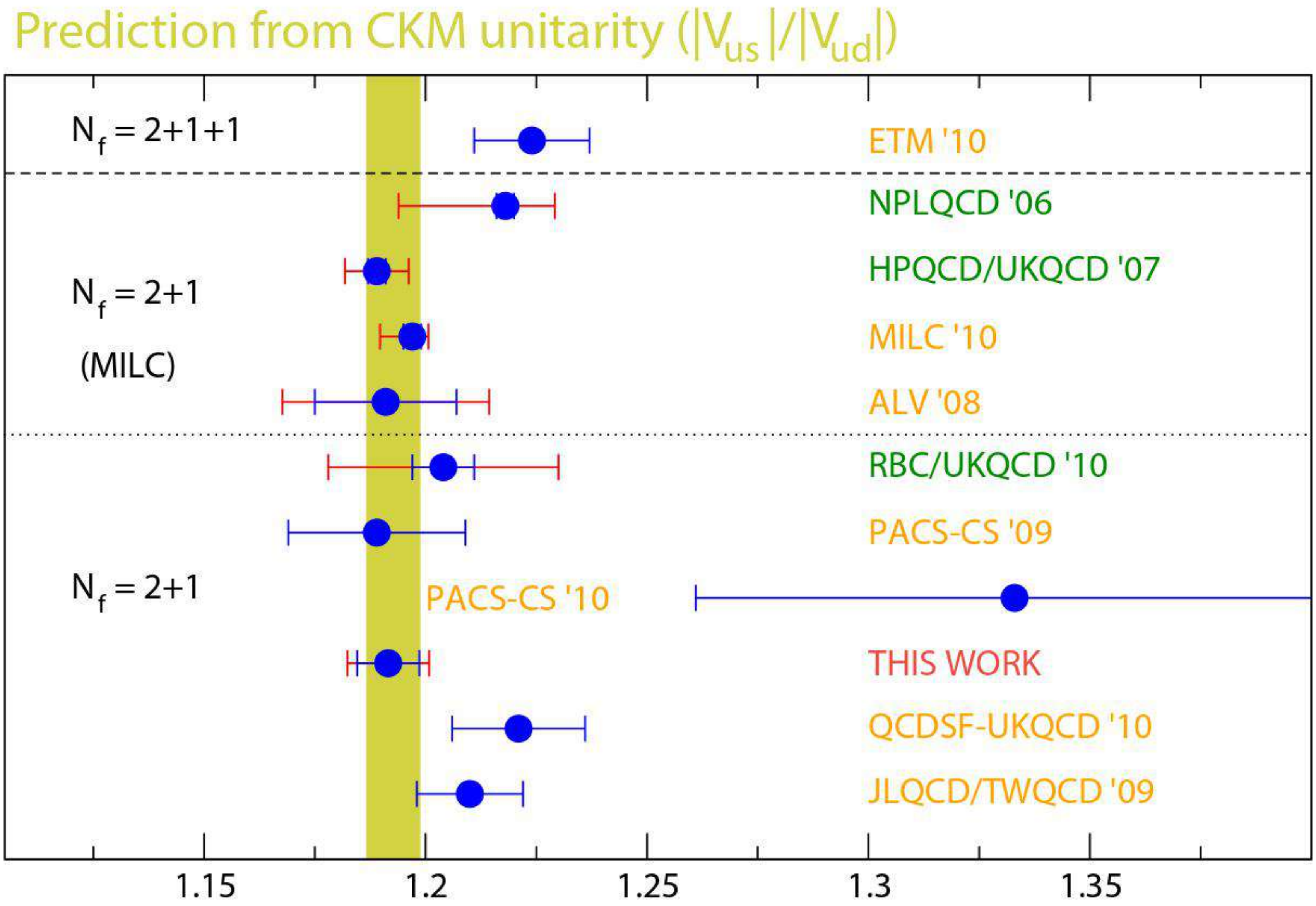
Method (ctd.):

- 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





f_K / f_π

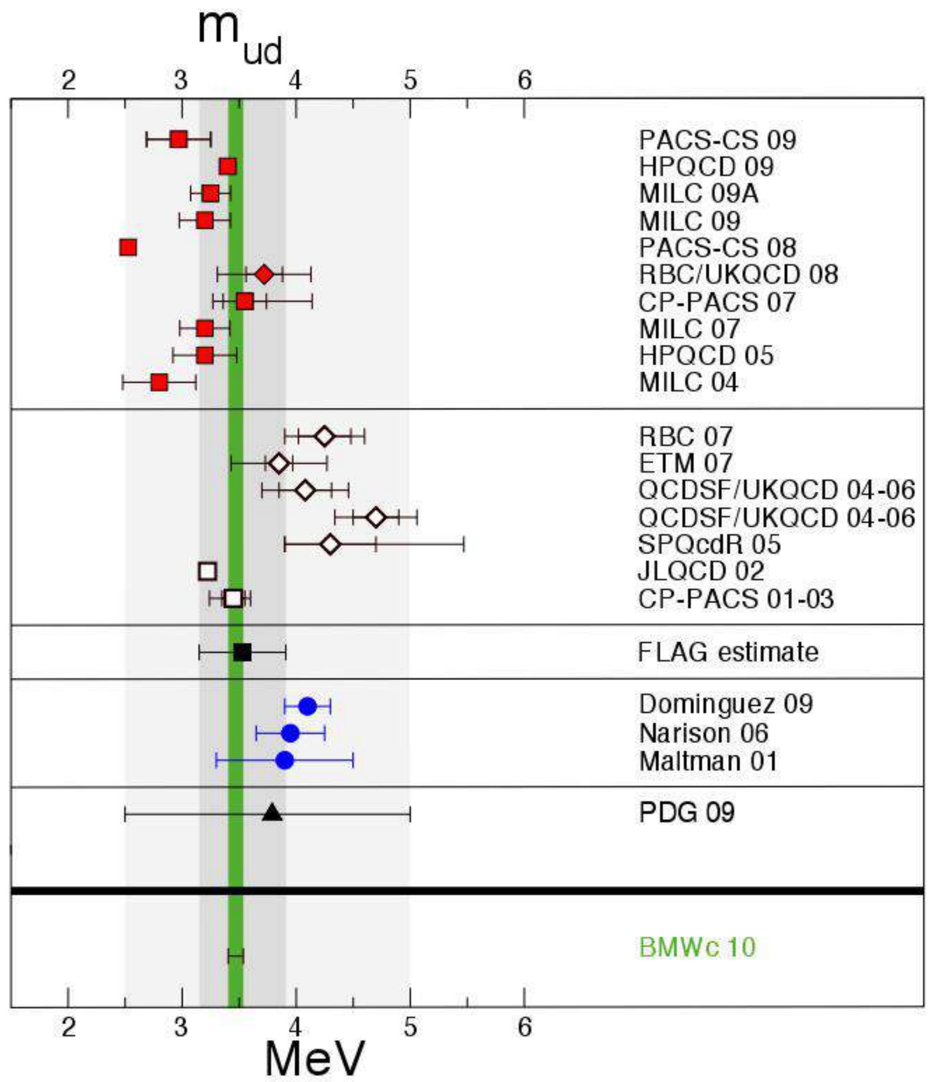

Prediction from CKM unitarity (|V_us|/|V_ud|)
N_f = 2+1+1
ETM '10
NPLQCD '06
HPQCD/UKQCD '07
N_f = 2+1
(MILC)
MILC '10
ALV '08
RBC/UKQCD '10
PACS-CS '09
N_f = 2+1
PACS-CS '10
THIS WORK
QCDSF-UKQCD '10
JLQCD/TWQCD '09
1.15
1.2
1.25
1.3
1.35

Individual m_u and m_d

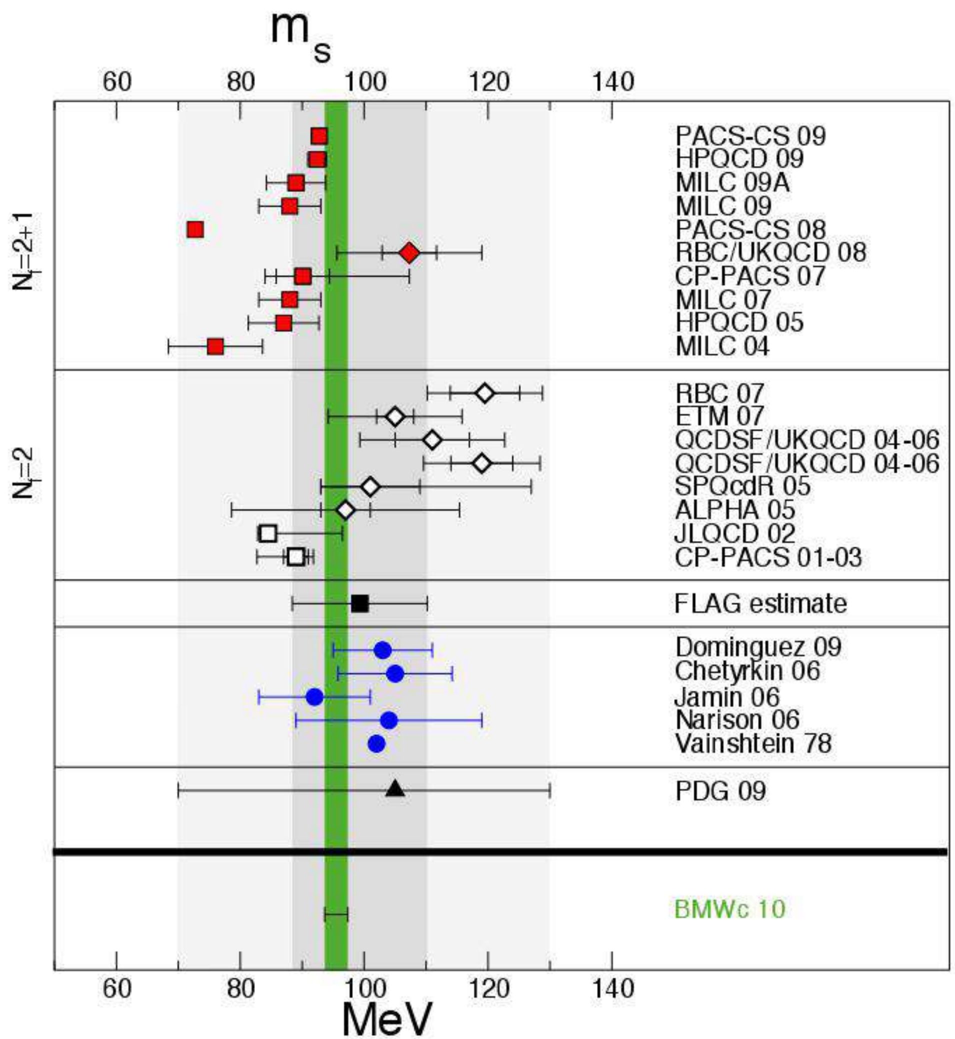
- Goal:
  - Compute m_u and m_d separately
- Method:
  - Need QED and isospin breaking effects in principle
  - Alternative: use dispersive input -Q from $\eta \to \pi\pi\pi$

    $Q^2 = \frac{1}{2}\left(\frac{m_s}{m_{ud}}\right)^2 \frac{m_d - m_u}{m_{ud}}$
  - ✓ Transform precise m_s/m_{ud} into $(m_d - m_u)/m_{ud}$
  - We use the conservative $Q = 22.3(8)$(Leutwyler, 2009)

Comparison

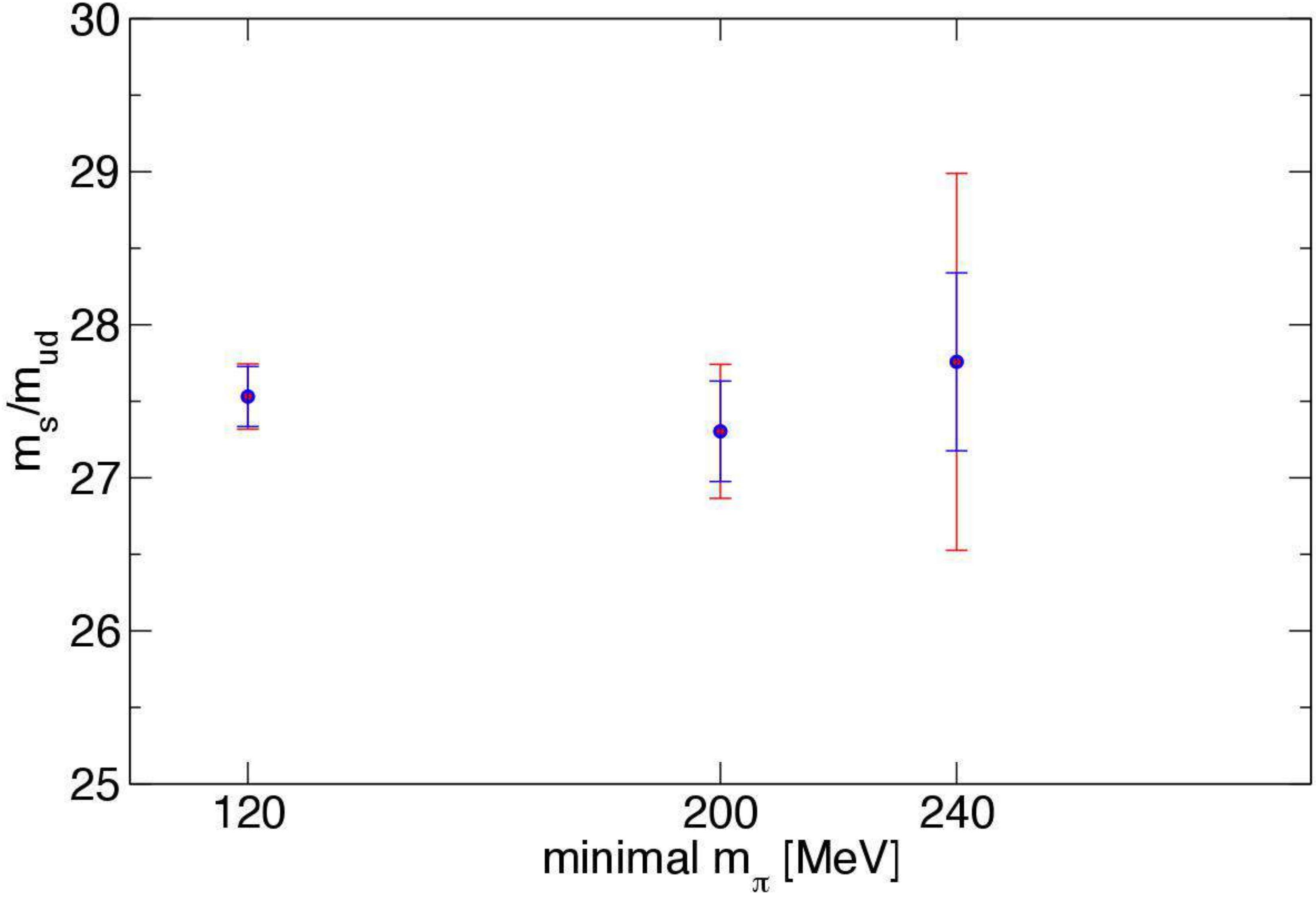


m_{ud}
2 3 4 5 6
PACS-CS 09
HPQCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPQCD 05
MILC 04
RBC 07
ETM 07
QCDSF/UKQCD 04-06
QCDSF/UKQCD 04-06
SPQcdR 05
JLQCD 02
CP-PACS 01-03
FLAG estimate
Dominguez 09
Narison 06
Maltman 01
PDG 09
BMWc 10
MeV

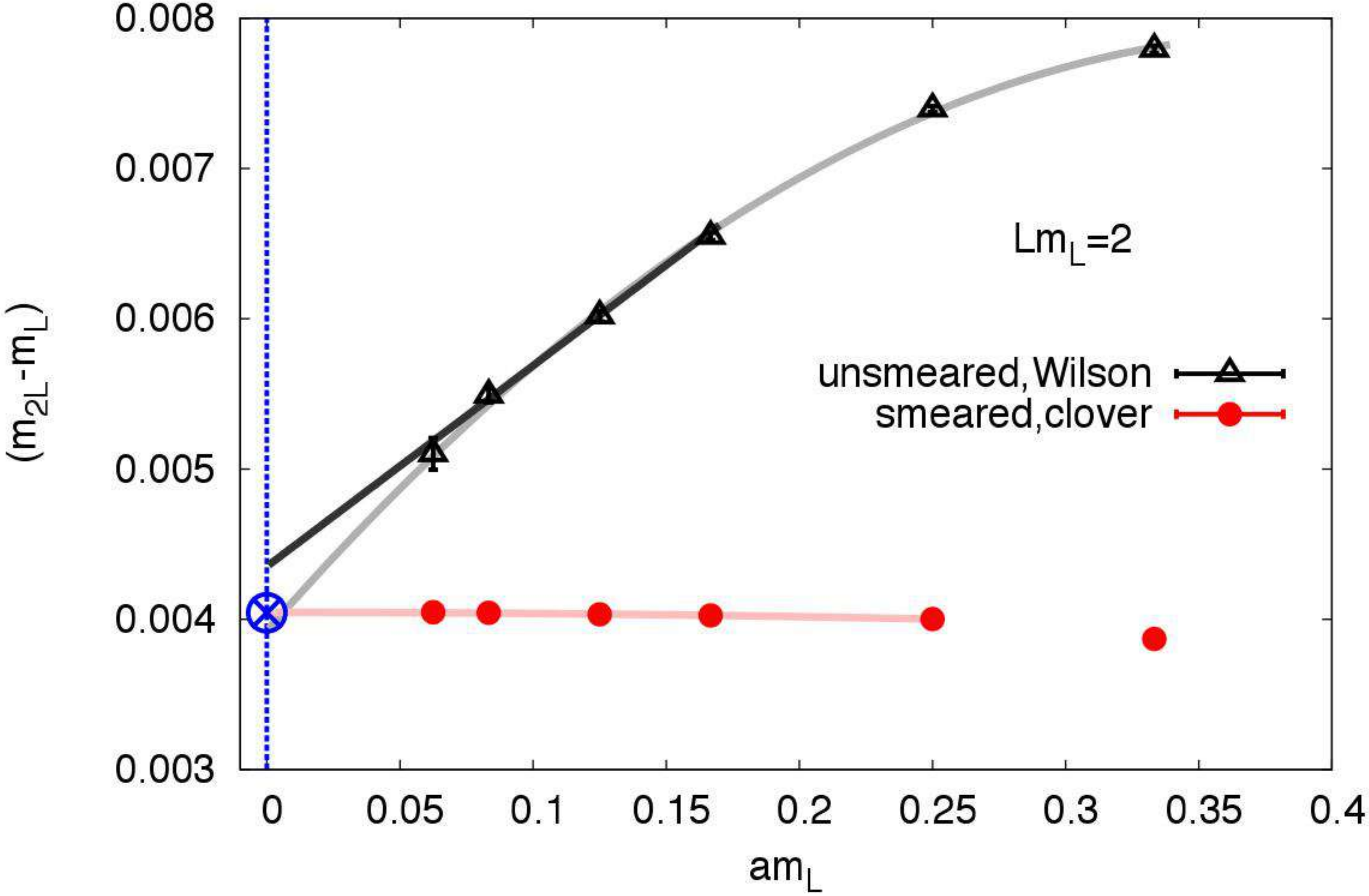


m_s
60 80 100 120 140
$N_f=2+1$
$N_f=2$
PACS-CS 09
HPQCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPQCD 05
MILC 04
RBC 07
ETM 07
QCDSF/UKQCD 04-06
QCDSF/UKQCD 04-06
SPQcdR 05
ALPHA 05
JLQCD 02
CP-PACS 01-03
FLAG estimate
Dominguez 09
Chetyrkin 06
Jamin 06
Narison 06
Vainshtein 78
PDG 09
BMWc 10
MeV

Chiral cuts



UV FILTERING



Moderate smearing (1 stout) improves scaling dramatically

Updating photon field

Long range QED interaction ➛ huge autocorrelation in standard HMC

- Solution: HMC in momentum space

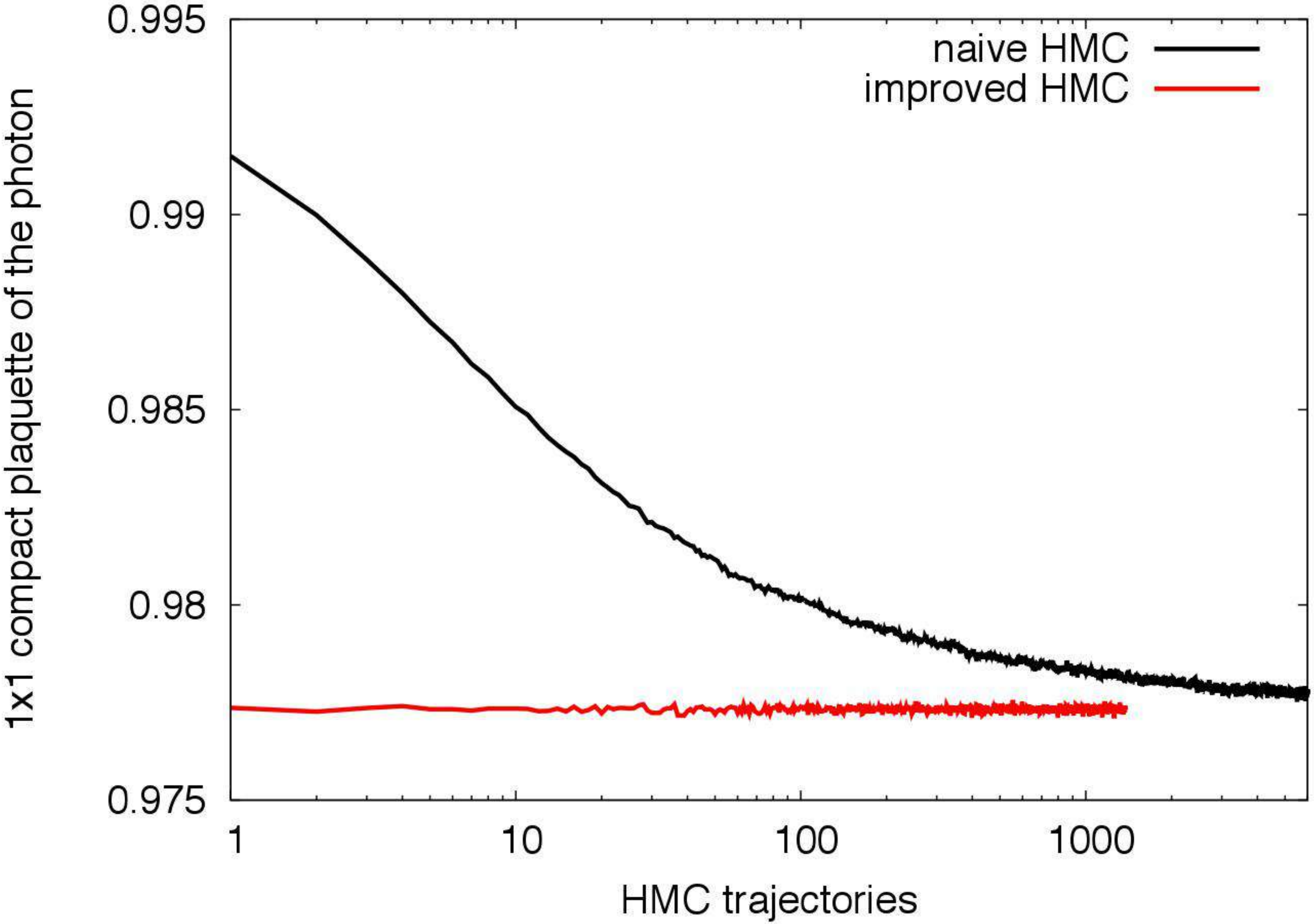
$$\mathcal{H} = \frac{1}{2V_4} \sum_{\mu,k} \left(|\hat{k}|^2 |A_\mu^k|^2 + \frac{|\Pi_\mu^k|^2}{m_k} \right)$$

- Use different masses per momentum

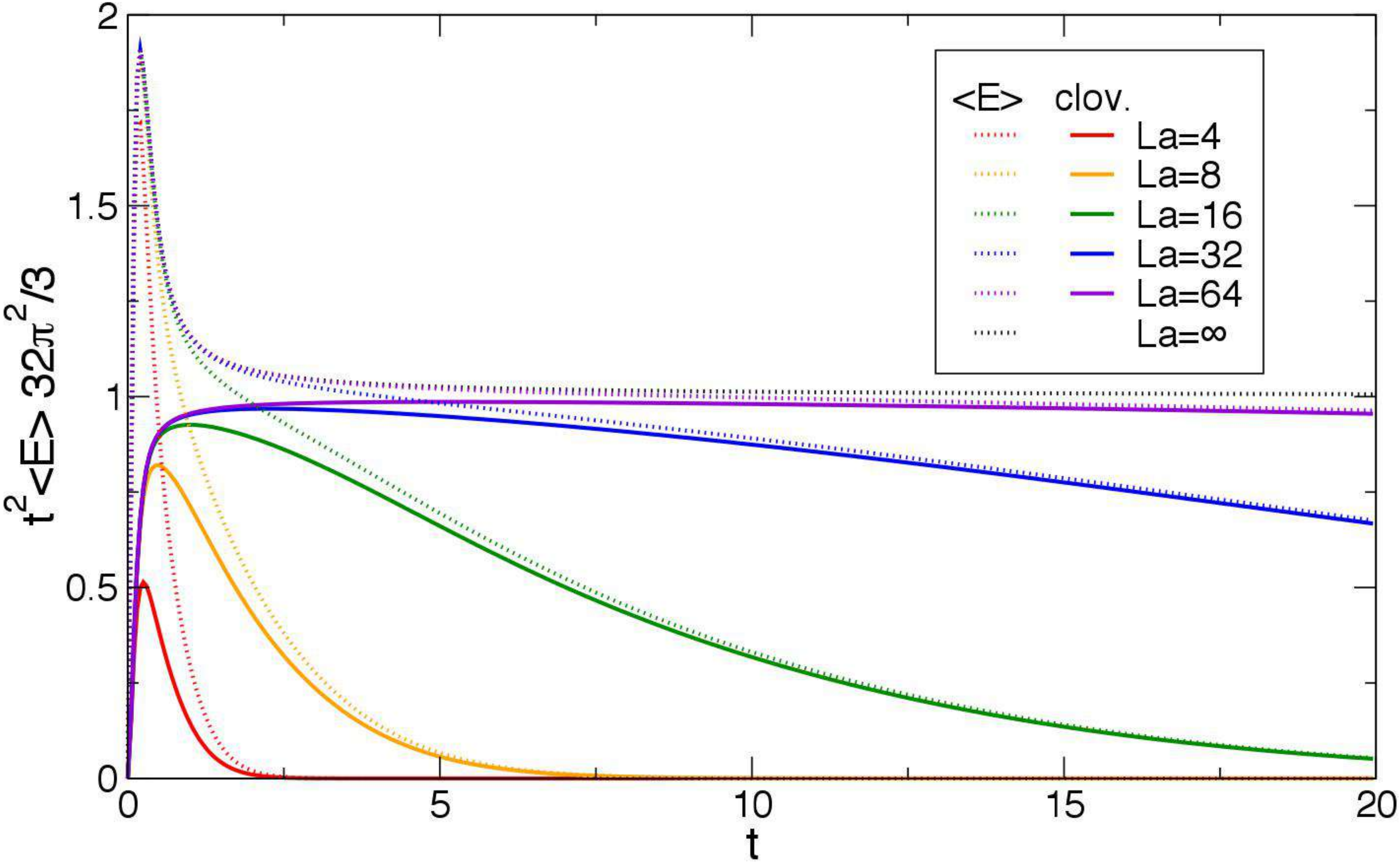
$$m_k = \frac{4|\hat{k}|^2}{\pi^2}$$

- Zero mode subtraction trivial
- Coupling to quarks in coordinate space ➛ FFT in every step

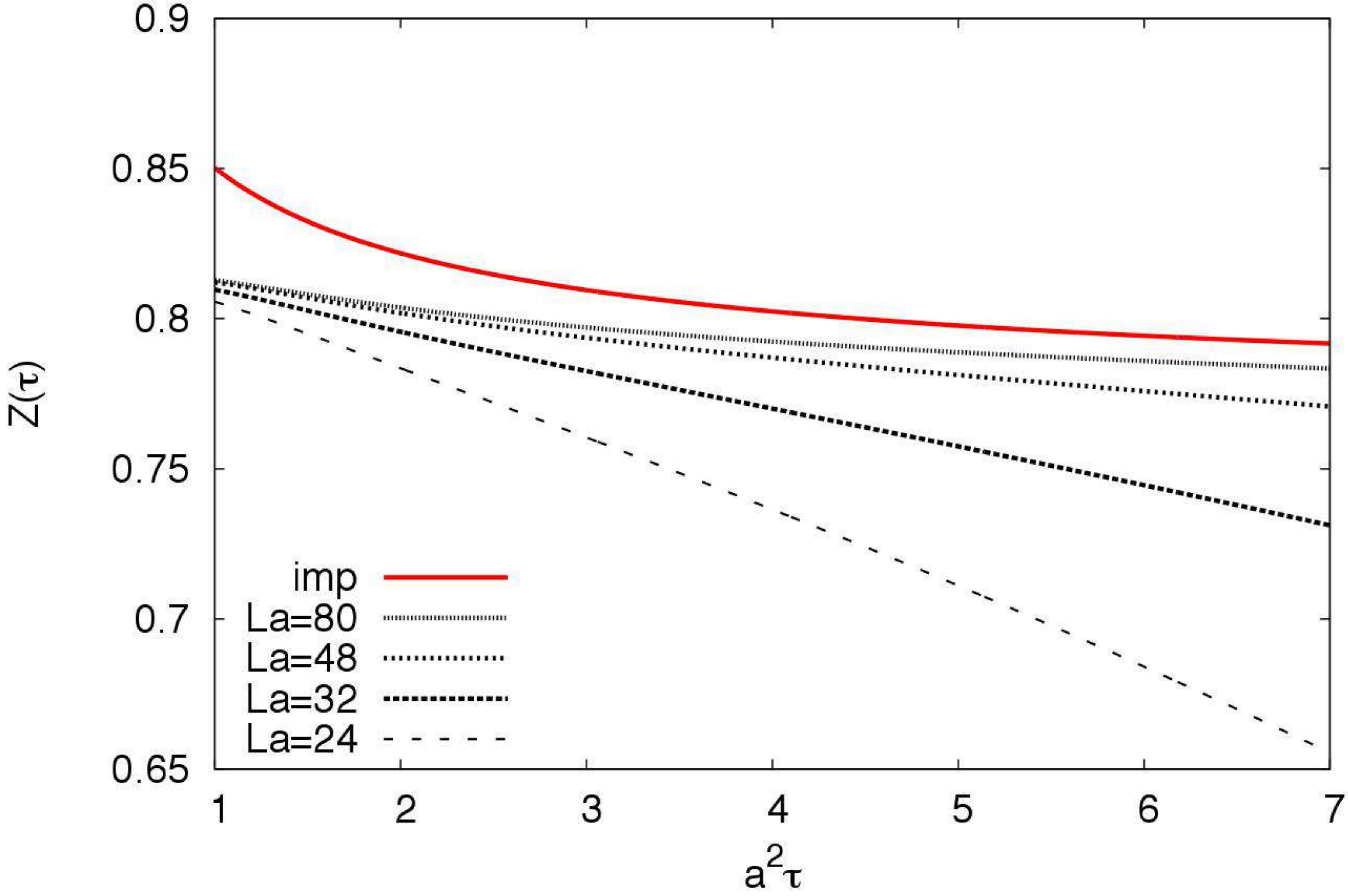
HMC FOR PHOTON FIELDS



TREE LEVEL CORRECTION



EFFECT OF TREE LEVEL CORRECTION



SCALING IN RENORMALISED COUPLING

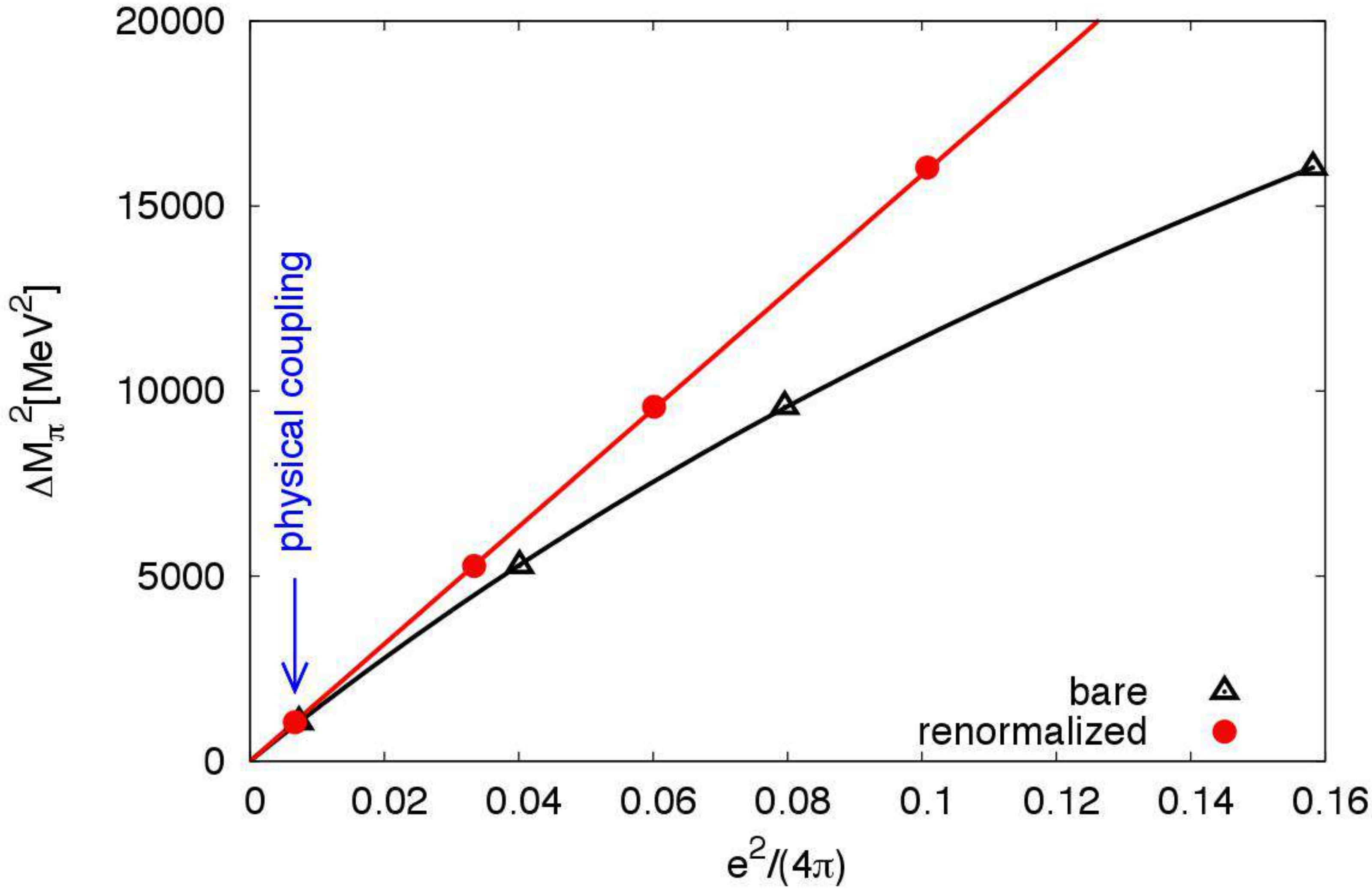


Illustration with precise $\Delta M_\pi^2 = M_{\bar{u}d}^2 - (M_{\bar{u}u}^2 + M_{\bar{d}d}^2)/2$

Combining results

How to determine the spread of results?

- Stdev or 1σ confidence interval of results
- Can weight it with fit quality Q

Information theoretic optimum: Akaike Information Criterion

- Information content of a fit depends on how well data are described per fit parameter
- Information lost wrt. correct fit $\propto$ cross-entropy J
- Compute information cross-entropy J_m of each fit m
- Probability that fit is correct $\propto e^{J_m}$

Akaike information criterion

- N measurments Γ_i from unknown pdf $g(\Gamma)$
- Fit model $f(\Gamma|\Theta)$ with parameters Θ
- Cross-entropy ($\sim$ Kullback-Leibler divergence)

$$J_m = J(g, f_m[\Theta]) = \int d\Gamma\, g(\Gamma) \ln(f(\Gamma|\Theta))$$

- For $N \to \infty$ and f close to g:

$$J_m = -\frac{\chi_m^2}{2} - p_m$$

where p_m is the number of fit parameters

Is this the only correct method?