# Quark masses from lattice QCD+QED

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Determination of the Fundamental Parameters in QCD
MITP, Mar. 9th, 2016

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SFB TR55

BERGISCHE UNIVERSITÄT WUPPERTAL

# How to compute quark masses?

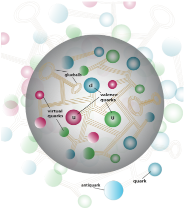
Problem:

- QCD fundamental degrees of freedom: quarks and gluons
- QCD observed objects: protons, neutrons ($\pi$, K, …)

☞Basic recipie:

- Solve QCD for various quark masses

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

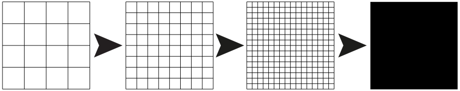



- Compare some results (e.g. $m_\pi, m_K, m_\Xi/m_\Omega$) with experiment
- Find quark masses that give correct physical results
- Renormalize

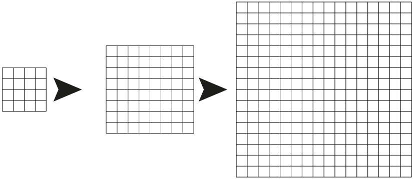
# Lattice

Lattice QCD=QCD when

- Cutoff removed (continuum limit)



- Infinite volume limit taken

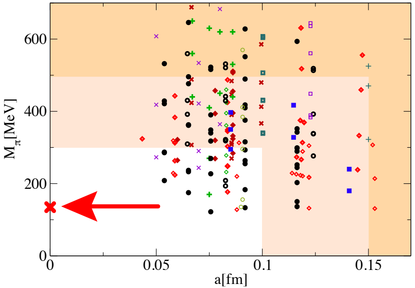


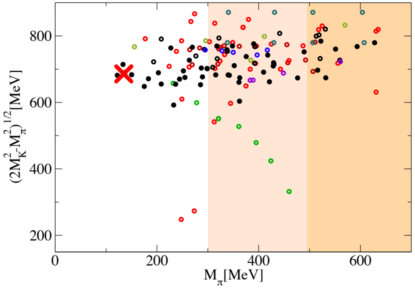
- At physical hadron masses (Especially $\pi$)
  - Numerically challenging to reach light quark masses

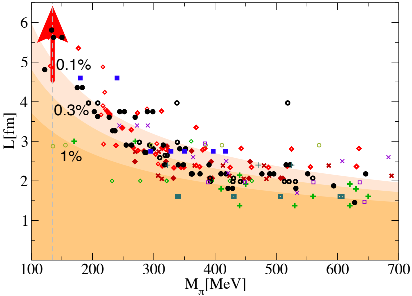
Statistical error from stochastic estimate of the path integral

# Extracting a physical prediction

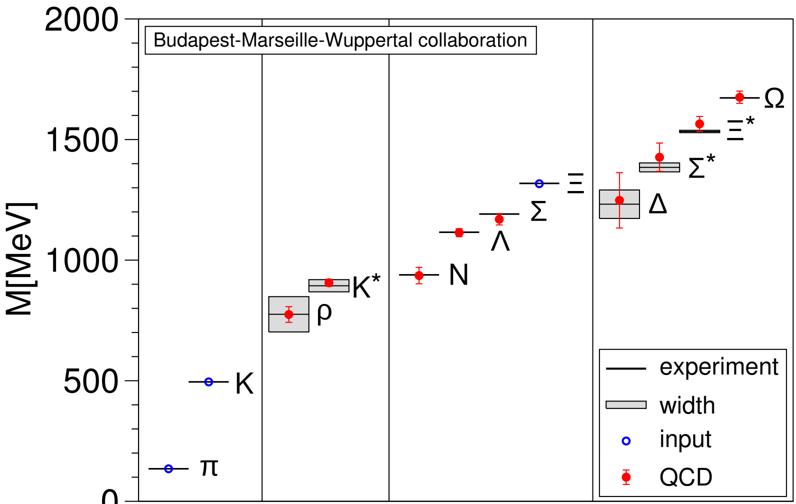
- Compute target observable
- Identify physical point
- Extrapolate to physical point



# The light hadron spectrum




(Science 322:1224,2008)

# Action details

Goal:

- Optimize physics results per CPU time
- Conceptually clean formulation

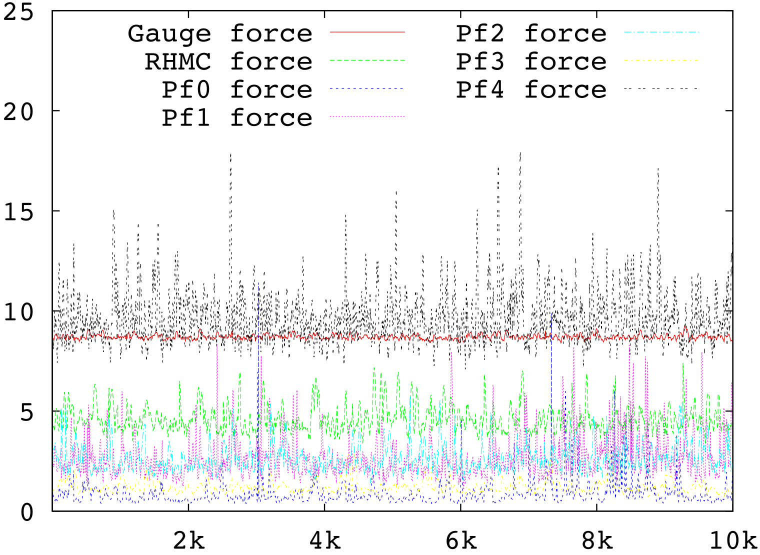
Method:

- Dynamical $2+1$ flavor, Wilson fermions at physical $M_\pi$
- 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)

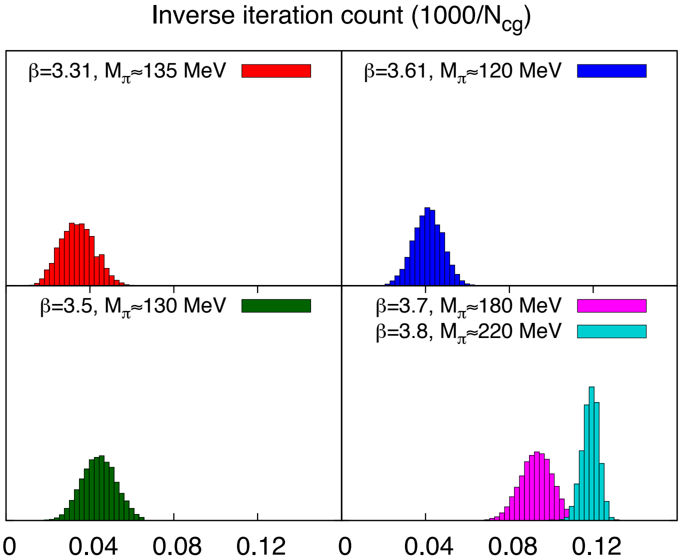
➢ Discretization effects of $O(\alpha_s a, a^2)$

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

# Algorithm stability

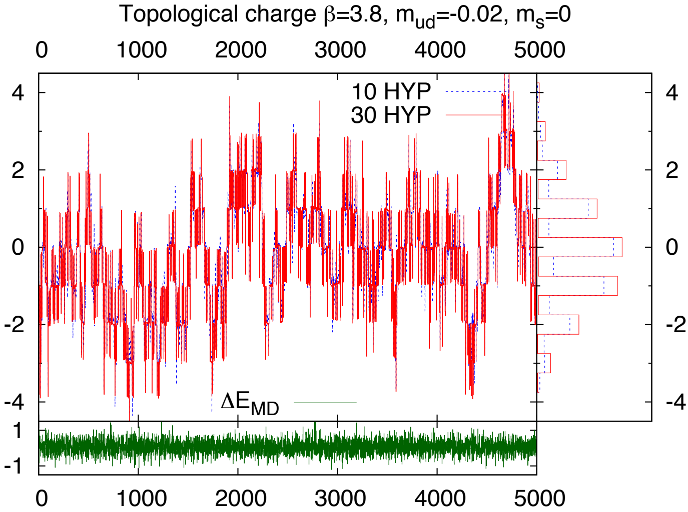


# No exceptional configs



# Topological sector sampling

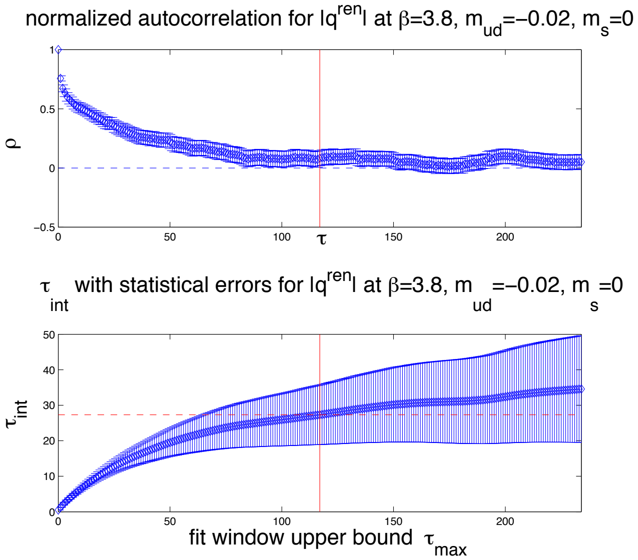
worst case



# Autocorrelation time (finest lattice, small mass)

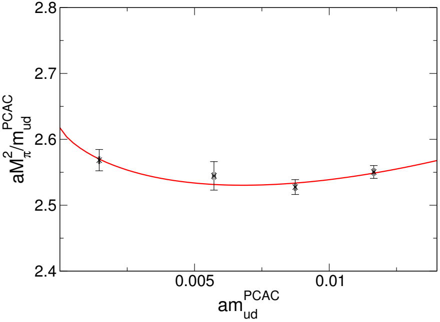
$\tau_{\text{int}} = 27.3(7.4)$

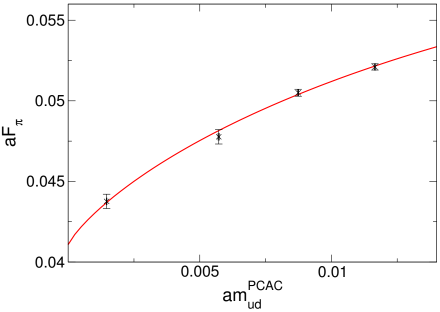
(MATLAB code from Wolff, 2004-7)



# Chiral interpolation

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




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

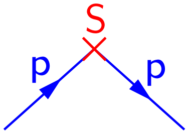
➢ We use $SU(2)$ $\chi$PT and Taylor interpolation forms

# Renormalization

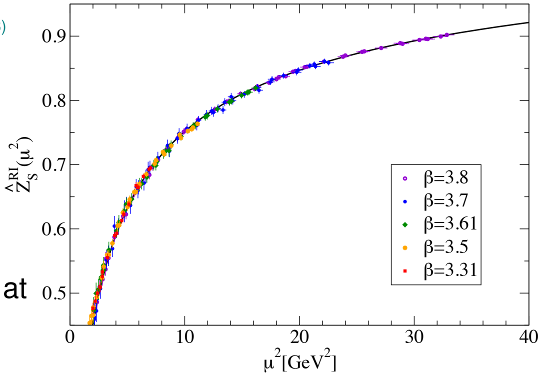
- Quark masses logarithmically divergent ($a \to 0$) ➛ renormalization
- Usual scheme $\overline{\text{MS}}$: perturbatively defined

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

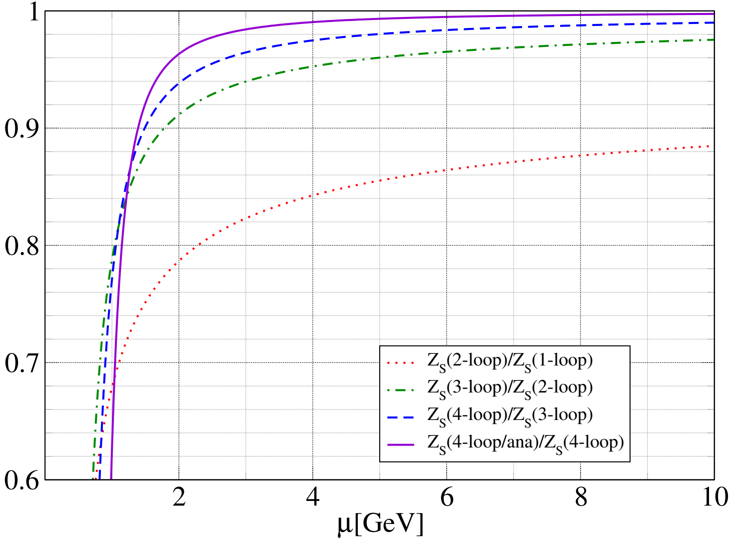
- Matrix elements of off-shell quarks in fixed gauge




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

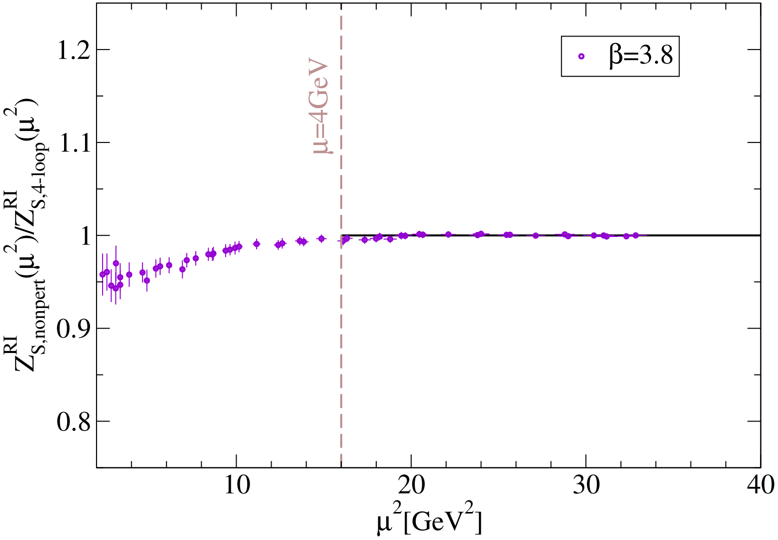


# Desired scale in RI-MOM scheme

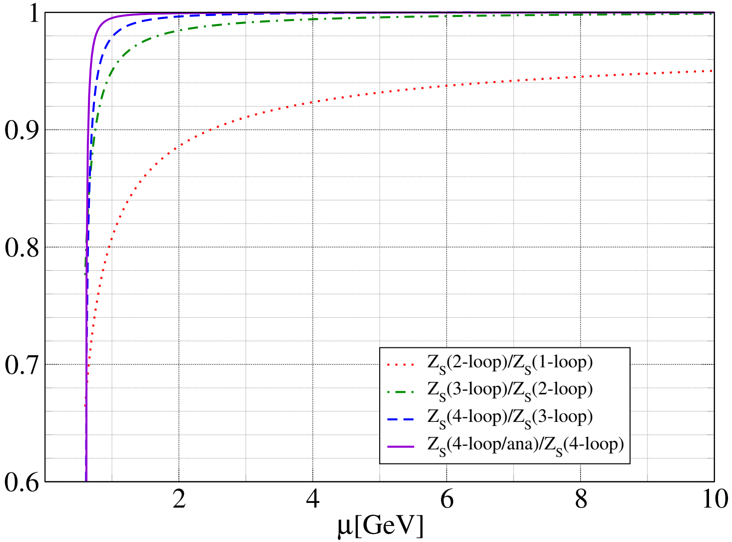



(Chetyrkin, Retey, 1999)

# Renormalization: contact with perturbation theory



# Optional conversion to $\overline{\mathrm{MS}}$




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

# Quark mass definitions

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

- $m^{\text{PCAC}}$ 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 $m_{\text{crit}}$

✓ Only $Z_S$ multiplicative renormalization (no pion poles)

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

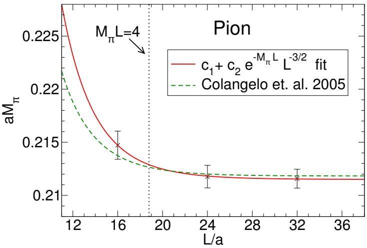
# Finite volume effects from virtual pions

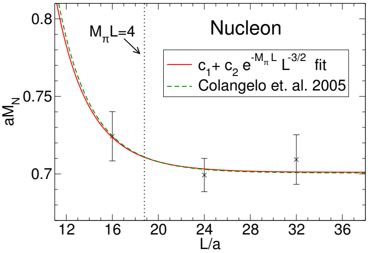
Goal:

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

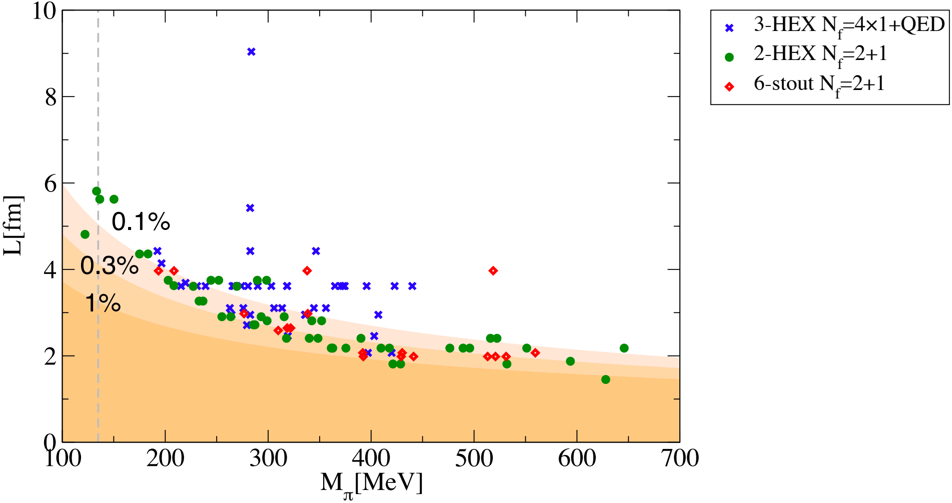
Method:

- 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)

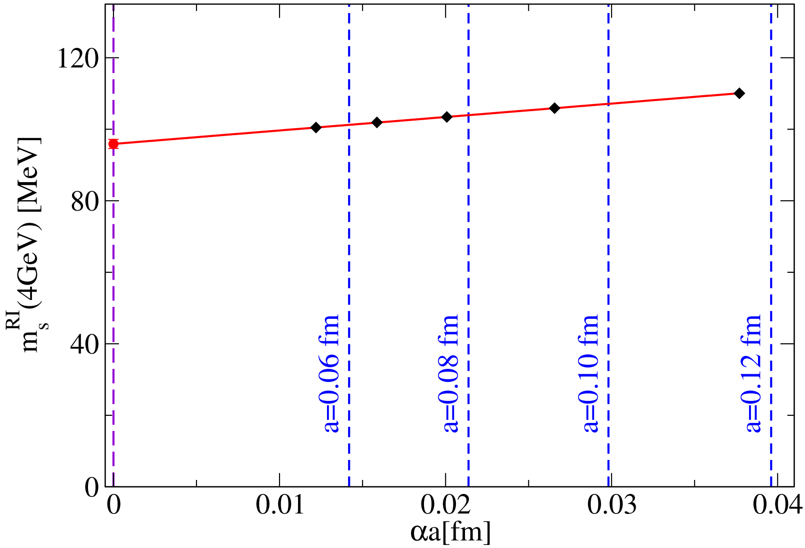


# Landscape $L$ vs. $M_\pi$



# Continuum limit



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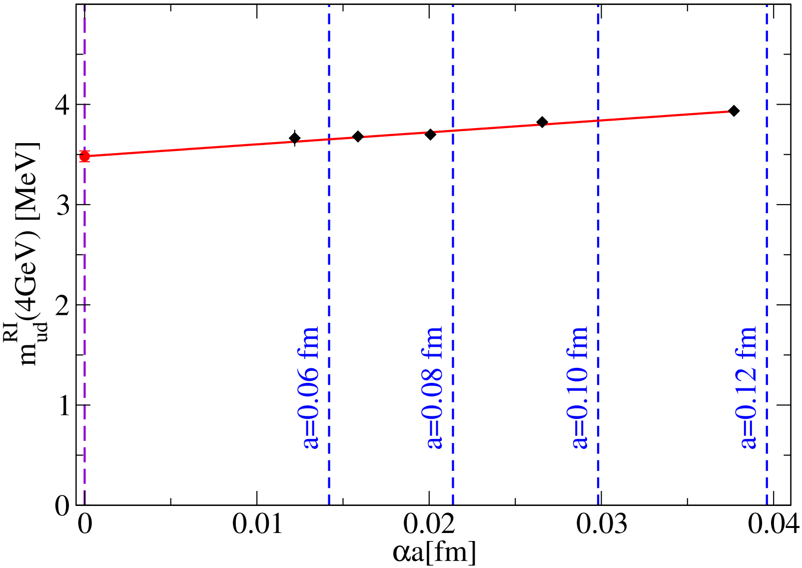

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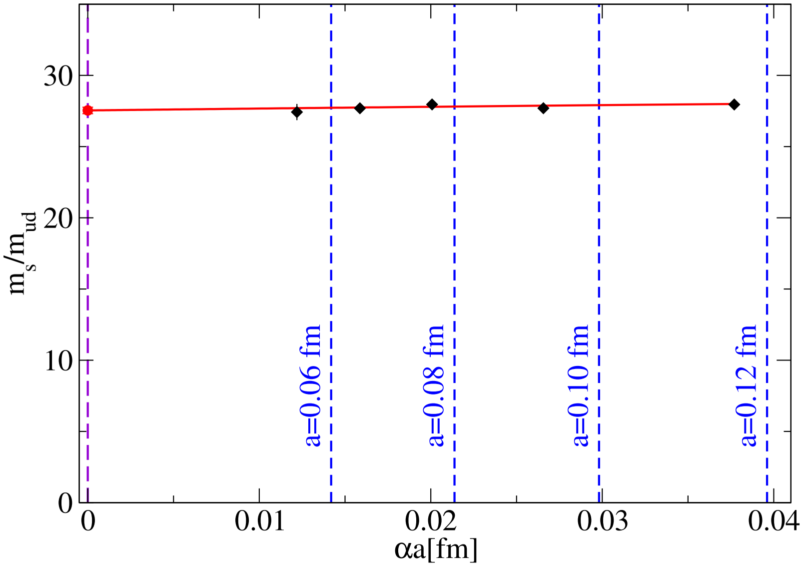
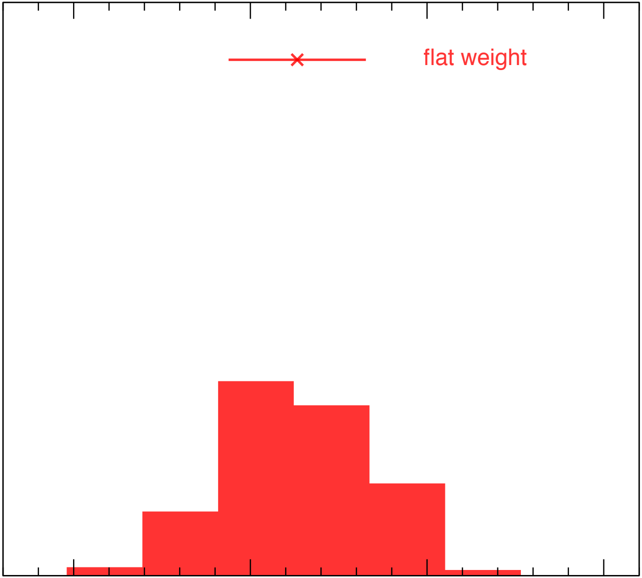


# Systematic error treatment

One conservative strategy for systematics:

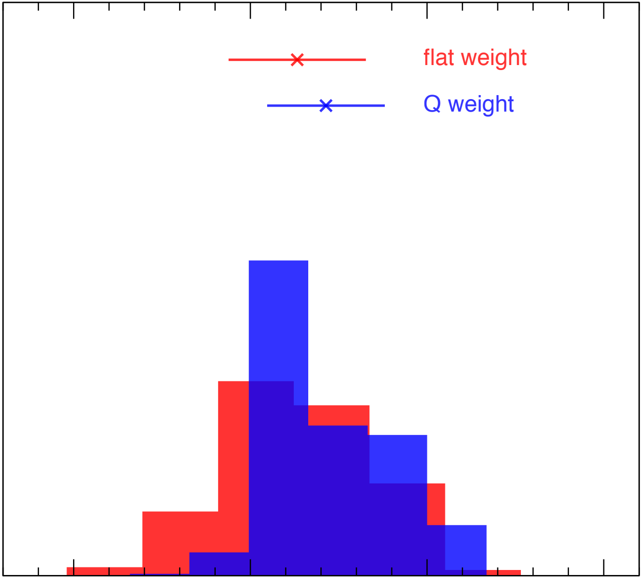
- Identify all higher order effects you have to neglect
- For each of them:
  - Repeat the entire analysis treating this one effect differently
  - Add the spread of results to systematics
- Important:
  - Do not do suboptimal analyses
  - Do not double-count analyses
- Error sources considered:
  - Plateaux range (Excited states)
  - $M_\pi$, $M_K$ 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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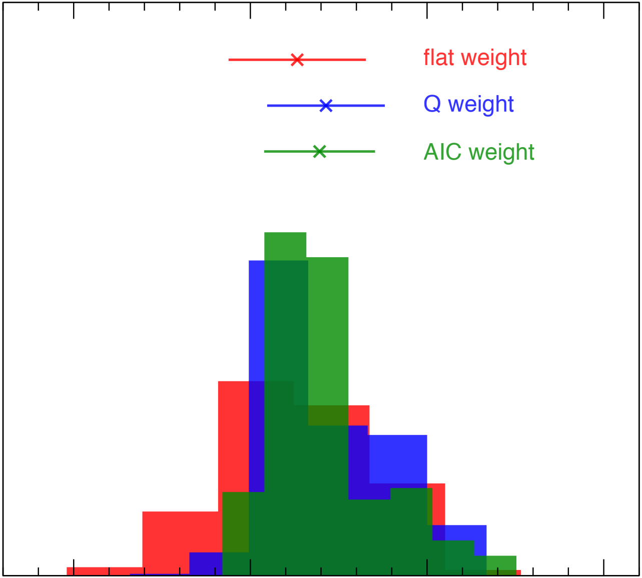



- Perform O(10000) analyses
- Difference: higher order effects
- Draw histogram of results
- Different weights possible
- Crosscheck agreement

# 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 |

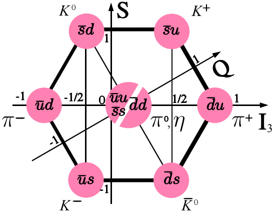
(JHEP 1108:148,2011; PLB 701:265,2011)

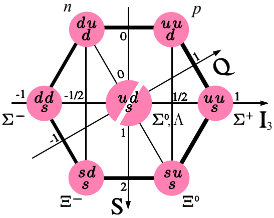
# Comparison

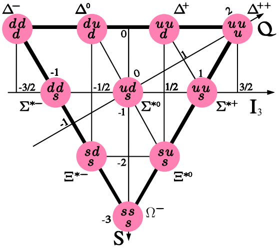
| Collaboration | Ref. | publication status | chiral extrapolation | continuum extrapolation | finite volume | renormalization | running | $m_{ud}$ | $m_s$ |
|---|---|---|---|---|---|---|---|---|---|
| RBC/UKQCD 12$^{\ominus}$ | [25] | A | ★ | ○ | ★ | ★ | $a$ | 3.37(9)(7)(1)(2) | 92.3(1.9)(0.9)(0.4)(0.8) |
| PACS-CS 12$^{\star}$ | [76] | A | ★ | ■ | ■ | ★ | $b$ | 3.12(24)(8) | 83.60(0.58)(2.23) |
| Laiho 11 | [77] | C | ○ | ★ | ★ | ○ | – | 3.31(7)(20)(17) | 94.2(1.4)(3.2)(4.7) |
| BMW 10A, 10B$^{+}$ | [22, 23] | A | ★ | ★ | ★ | ★ | $c$ | 3.469(47)(48) | 95.5(1.1)(1.5) |
| PACS-CS 10 | [21] | A | ★ | ■ | ■ | ★ | $b$ | 2.78(27) | 86.7(2.3) |
| MILC 10A | [75] | C | ○ | ★ | ★ | ○ | – | 3.19(4)(5)(16) | – |
| HPQCD 10$^{*}$ | [73] | A | ○ | ★ | ★ | – | – | 3.39(6) | 92.2(1.3) |
| RBC/UKQCD 10A | [78] | A | ○ | ○ | ★ | ★ | $a$ | 3.59(13)(14)(8) | 96.2(1.6)(0.2)(2.1) |
| Blum 10$^{\dagger}$ | [32] | A | ○ | ■ | ○ | ★ | – | 3.44(12)(22) | 97.6(2.9)(5.5) |
| PACS-CS 09 | [20] | A | ★ | ■ | ■ | ★ | $b$ | 2.97(28)(3) | 92.75(58)(95) |
| HPQCD 09A$^{\oplus}$ | [72] | A | ○ | ★ | ★ | – | – | 3.40(7) | 92.4(1.5) |
| MILC 09A | [37] | C | ○ | ★ | ★ | ○ | – | 3.25 (1)(7)(16)(0) | 89.0(0.2)(1.6)(4.5)(0.1) |
| MILC 09 | [15] | A | ○ | ★ | ★ | ○ | – | 3.2(0)(1)(2)(0) | 88(0)(3)(4)(0) |
| PACS-CS 08 | [19] | A | ★ | ■ | ■ | ■ | – | 2.527(47) | 72.72(78) |
| RBC/UKQCD 08 | [79] | A | ○ | ■ | ★ | ★ | – | 3.72(16)(33)(18) | 107.3(4.4)(9.7)(4.9) |
| CP-PACS/ JLQCD 07 | [80] | A | ■ | ★ | ★ | ■ | – | 3.55(19)($^{+56}_{-20}$) | 90.1(4.3)($^{+16.7}_{-4.3}$) |
| HPQCD 05 | [81] | A | ○ | ○ | ○ | ○ | – | 3.2(0)(2)(2)(0)$^{\ddagger}$ | 87(0)(4)(4)(0)$^{\ddagger}$ |
| MILC 04, HPQCD/ MILC/UKQCD 04 | [36, 82] | A | ○ | ○ | ○ | ■ | – | 2.8(0)(1)(3)(0) | 76(0)(3)(7)(0) |

(FLAG, 2013)

# 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

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

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

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

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

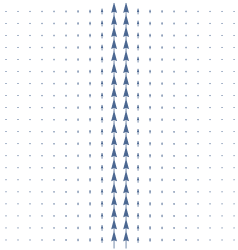
Method 2: direct calculation

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

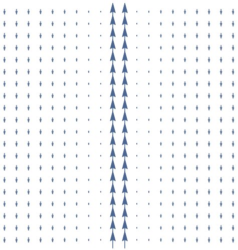
# Challenges of QED simulations

- Effective theory only (UV completion unclear)
- $\pi^+$, $p$, 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

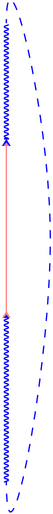
➢ Keep it non-compact (no problem with topology in 4D-$U(1)$)

- 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

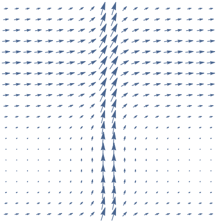
- Removing momentum modes with measure 0 as $V \to \infty$ allowed
- Remove $k = 0$ from momentum sum ($QED_{TL}$)
  - Realised by a constraint term in the action

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

  - Couples all times ➛ no transfer matrix!
- Remove $\vec{k} = 0$ from momentum sum ($QED_L$)
  - Realised by a constraint term in the action

$$\lim_{\xi(t) \to 0} \int dt \frac{1}{\xi(t)} \left( \int d^3 x A_\mu(x) \right)^2$$

  - Transfer matrix exists



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

# Momentum subtraction

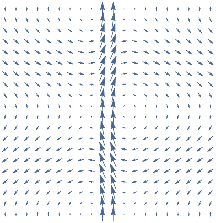
- Removing momentum modes with measure 0 as $V \to \infty$ allowed
- Remove $k = 0$ from momentum sum ($QED_{TL}$)
  - Realised by a constraint term in the action

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

  - Couples all times ➛ no transfer matrix!
- Remove $\vec{k} = 0$ from momentum sum ($QED_L$)
  - Realised by a constraint term in the action

$$\lim_{\xi(t) \to 0} \int dt \frac{1}{\xi(t)} \left( \int d^3 x A_\mu(x) \right)^2$$

  - Transfer matrix exists



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

# Momentum subtraction

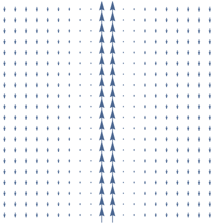
- Removing momentum modes with measure 0 as $V \to \infty$ allowed
- Remove $k = 0$ from momentum sum ($QED_{TL}$)
  - Realised by a constraint term in the action

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

  - Couples all times ➛ no transfer matrix!
- Remove $\vec{k} = 0$ from momentum sum ($QED_L$)
  - Realised by a constraint term in the action

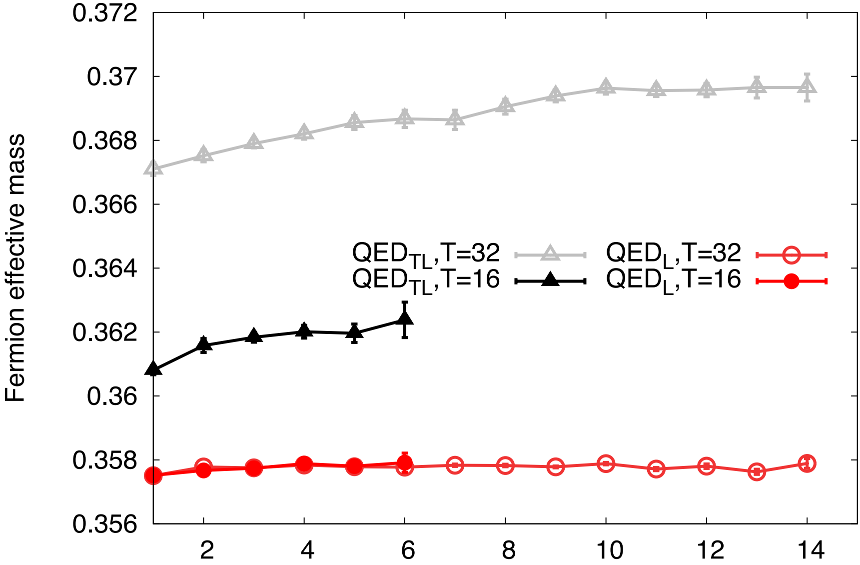
$$\lim_{\xi(t) \to 0} \int dt \frac{1}{\xi(t)} \left( \int d^3 x A_\mu(x) \right)^2$$

  - Transfer matrix exists



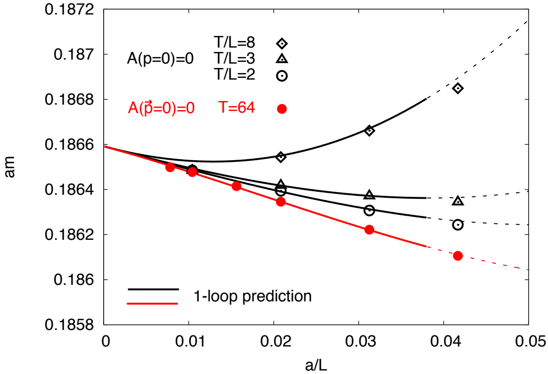
- Gauge fields unaffected in $QED_{TL}$, only Polyakov loops

# Quenched QED FV effects



# Finite volume subtraction

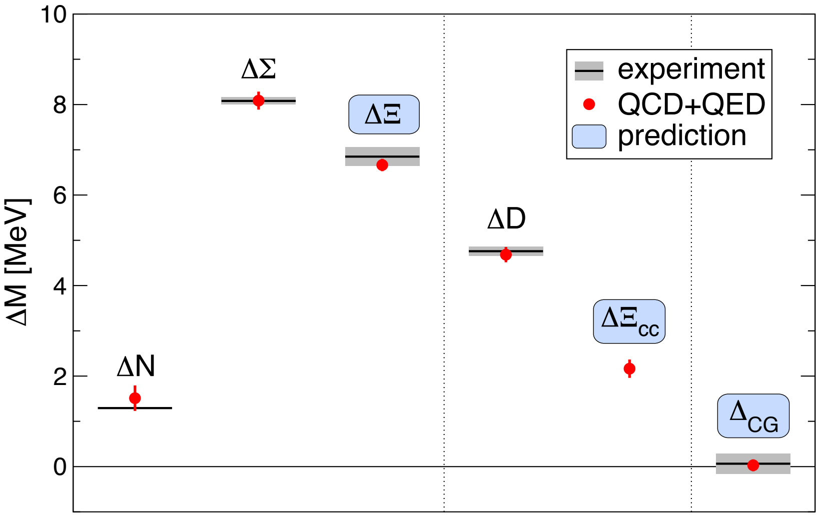
- Universal to $O(1/L^2)$
- Compositmess at $1/L^3$
- Fit $O(1/L^3)$
- Divergent $T$ dependence for $p = 0$ mode subtraction
- No $T$ dependence for $\vec{p} = 0$ mode subtraction




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

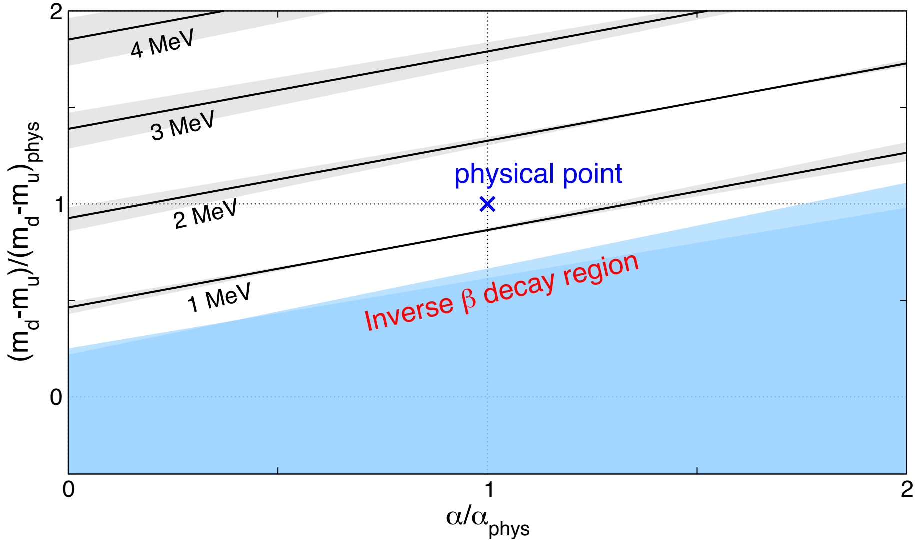
(BMWc, 2014)

# Hadronic isospin splitting

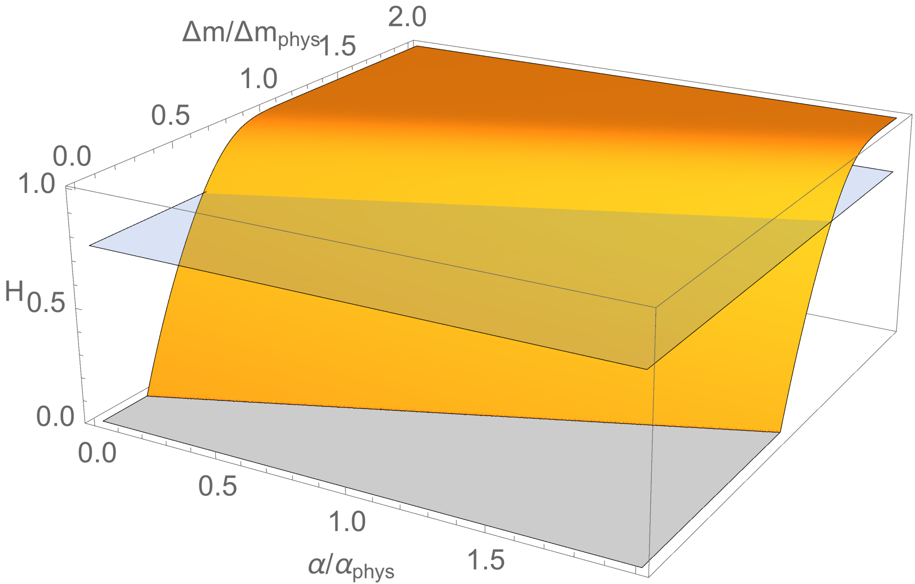



(BMWc 2014)

# Nucleon splitting QCD and QED parts



# Resulting initial hydrogen abundance



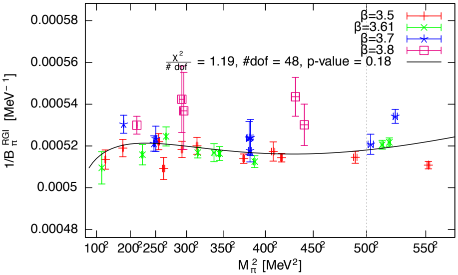
# Masses uf the $u$ and $d$ quarks

Goal:

- Directly compute $m_u$ and $m_d$

Method:

- Results in qQED as a first step
- Full QED: work in progress



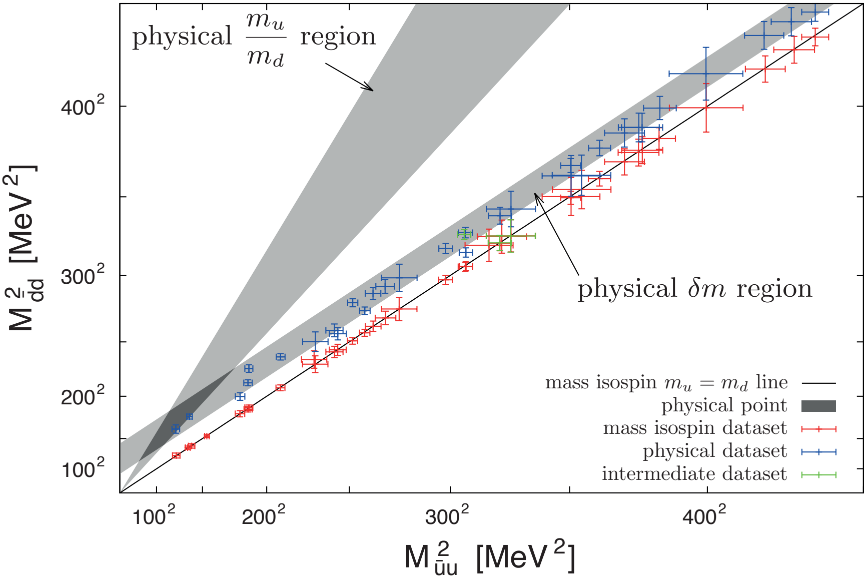

Computing $m_u - m_d$:

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

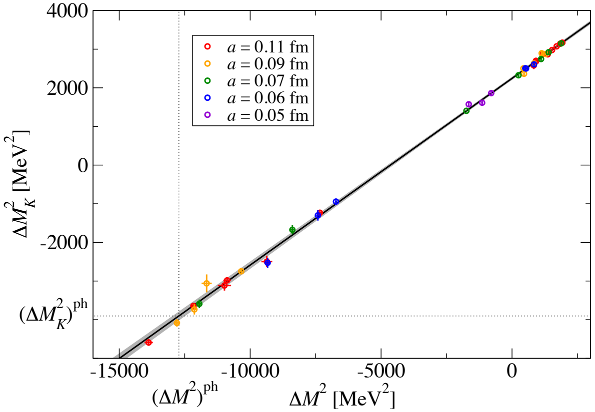
$$\Delta M^2 = 2B_2\delta m + O(m_{ud}\alpha, m_{ud}\delta m, \alpha^2, \alpha\delta m, \delta m^2)$$

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

# Extracting physical $\Delta M^2$

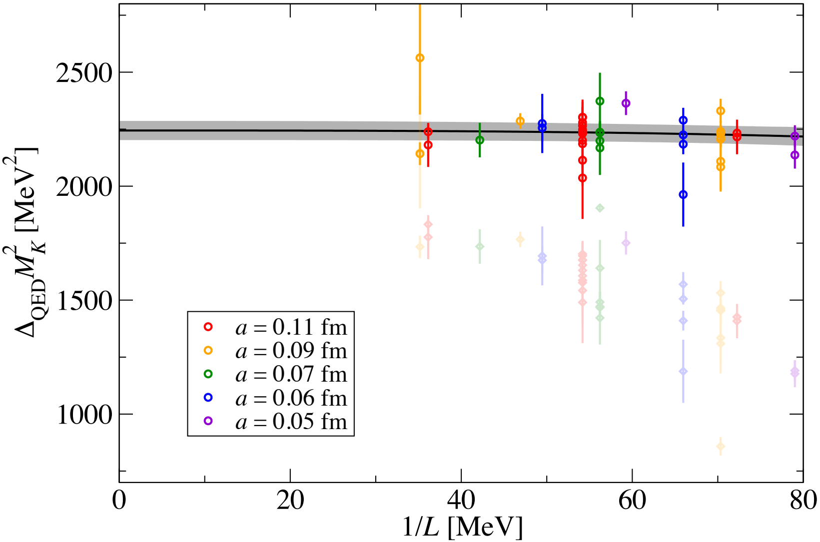



$$\Delta M_K^2 = \Delta M^2 C_X + \alpha D_X$$

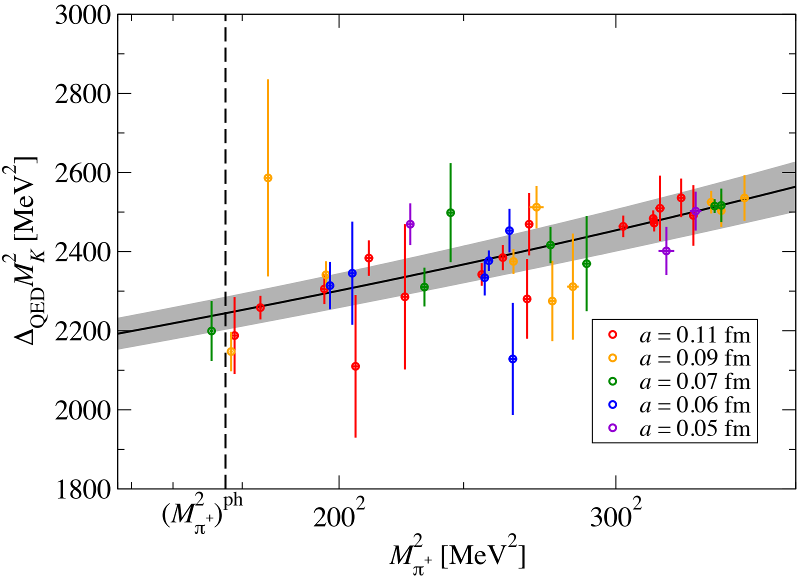
$$C_X = c_X^0 + c_X^1 \hat{M}_\pi^2 + c_X^2 \hat{M}_K^2 + c_X^3 f(a)$$

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

# Finite volume



# Chiral interpolation



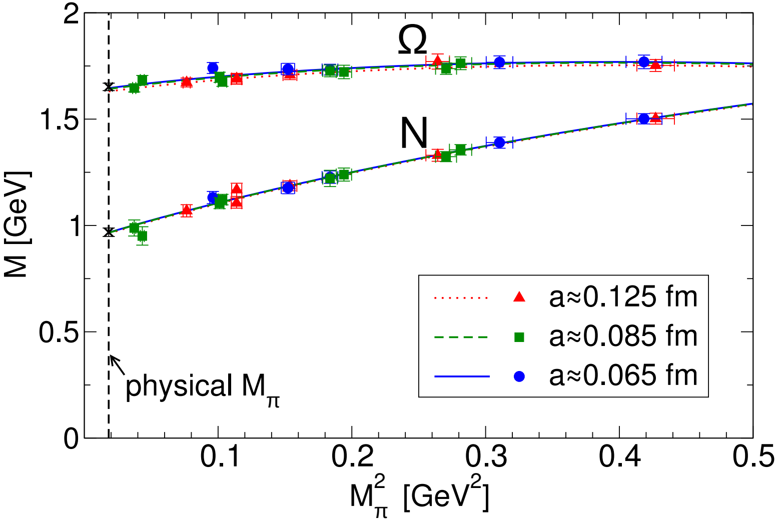
# Preliminary results

- $\delta m^{\overline{MS}}(2\text{GeV}) = -2.39(7)(6)(9)\text{MeV}$
- $m_u^{\overline{MS}}(2\text{GeV}) = 2.27(6)(6)(4)\text{MeV}$
- $m_d^{\overline{MS}}(2\text{GeV}) = 4.67(6)(6)(4)\text{MeV}$
- $m_u/m_d = 0.49(1)(1)(1)$

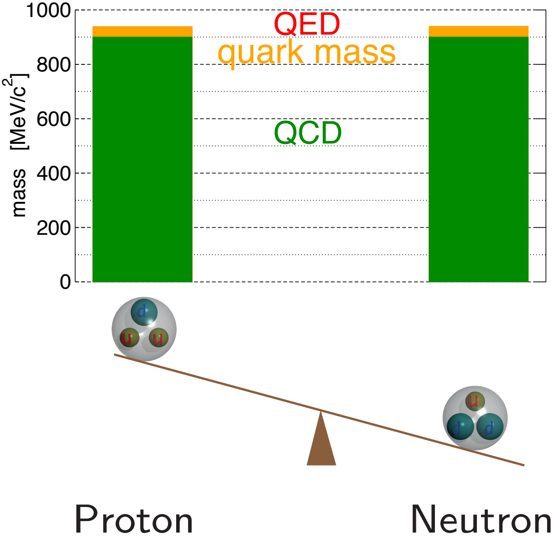
- $\epsilon := \frac{\Delta_{\text{QED}} M_K^2 - \Delta_{\text{QED}} M_\pi^2}{\Delta M_\pi^2} = 0.78(3)(7)(17)(2)$
- $R := \frac{m_s - m_{ud}}{m_d - m_u} = 38.5(1.3)(1.0)(1.4)$
- $R := \sqrt{\frac{m_s^2 - m_{ud}^2}{m_d^2 - m_u^2}} = 23.4(0.4)(0.3)(0.4)$

BACKUP

# Chiral continuum fit



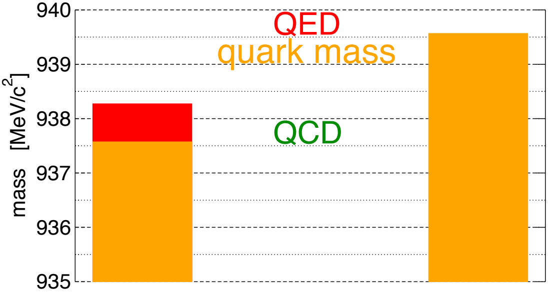
# Is the fine structure relavant?

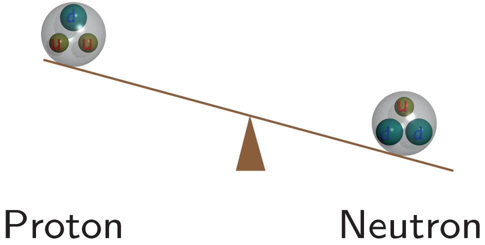



- Proton, neutron: 3 quarks
- Proton: uud
- Neutron: udd

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

# Is the fine structure relavant?

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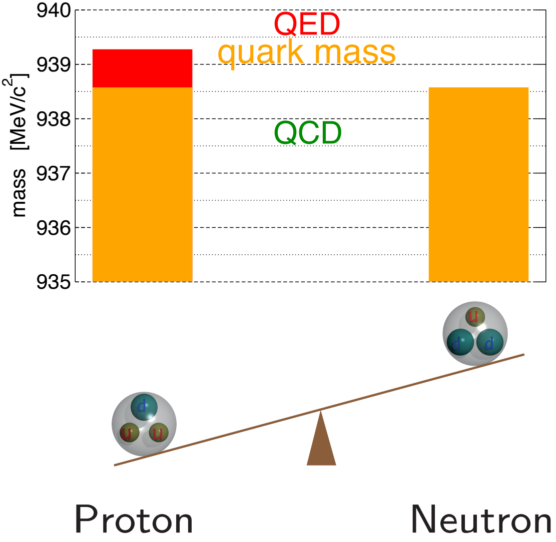


- Proton, neutron: 3 quarks
- Proton: uud
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- $m_u < m_d : M_p < M_n$
- $m_u = m_d : M_p > M_n$
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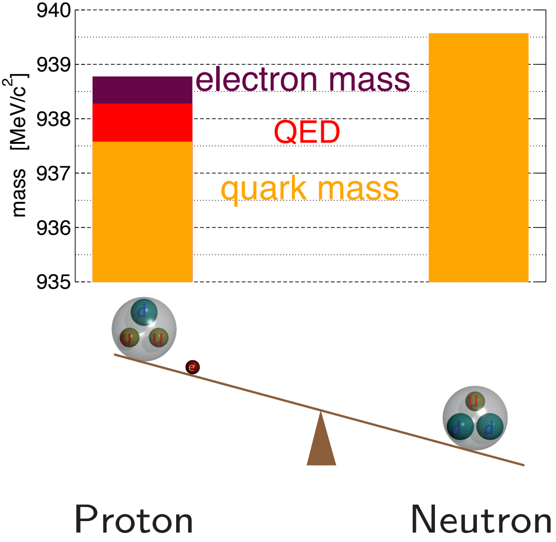
  No hydrogen

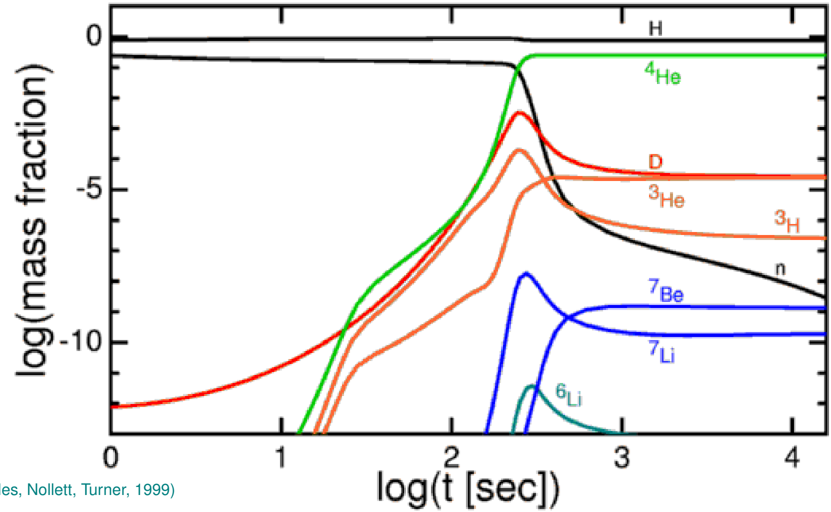
# Is the fine structure relavant?




- 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

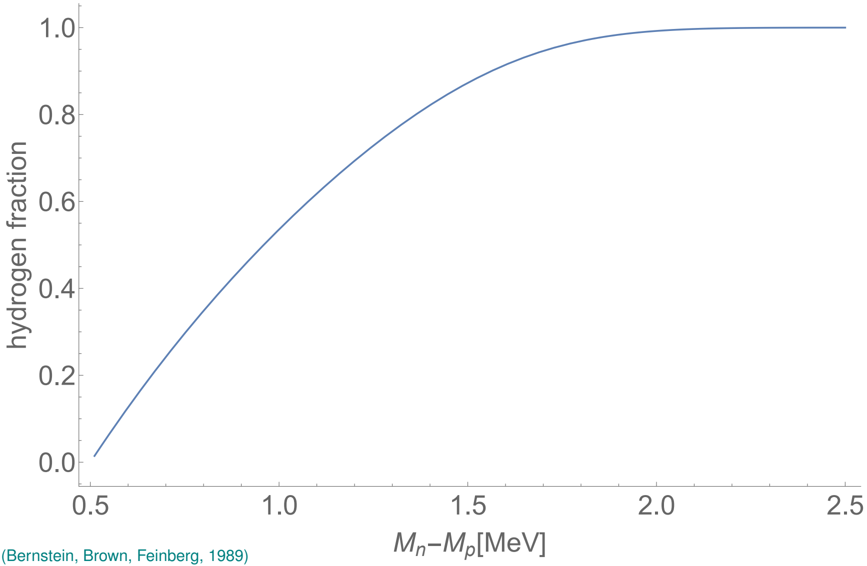
# Big bang nucleosynthesis




(Burles, Nollett, Turner, 1999)

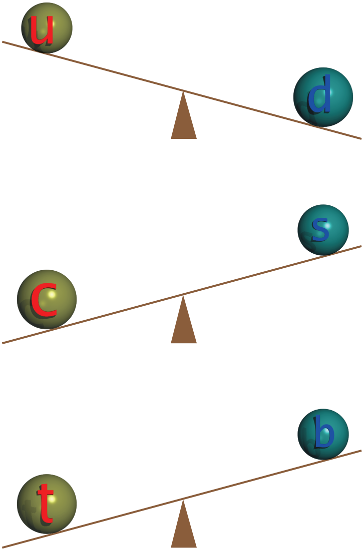
$M_n - M_p$ determines deuterium bottleneck

# Hydrogen abundance




(Bernstein, Brown, Feinberg, 1989)

# The light up quark

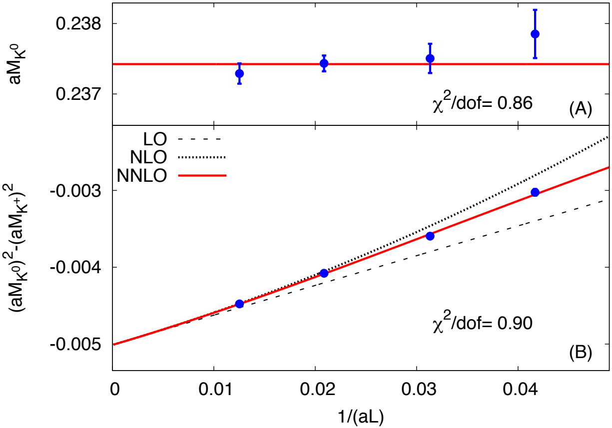



1st generation: $m_u < m_d$ Why?

2nd generation: $m_c > m_s$

3rd generation: $m_t > m_b$

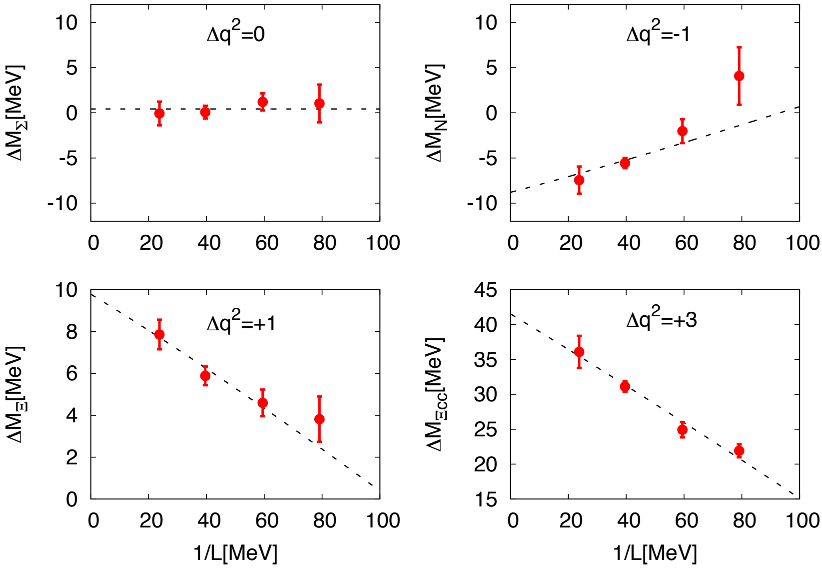
# Universal FV effects




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

(BMWc, 2014)

# Baryon FV in QCD+QED



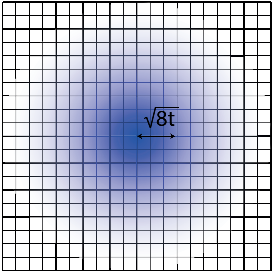
# Identifying the physical point

We need to fix 6 parameters: $m_u$, $m_d$, $m_s$, $m_c$,, $\alpha_s$ and $\alpha$

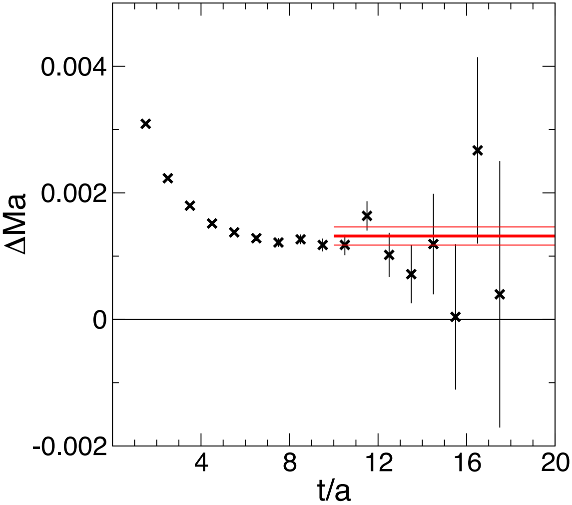
- Requires fixing 5 dimensionless ratios from 6 lattice observables
- 4 "canonical" lattice observables: $M_{\pi^\pm}$, $M_{K^+}$, $M_\Omega$, $M_D$
- Strong isospin splitting from $M_{K^\pm} - M_{K^0}$
- what about $\alpha$?
  - ✗ From $M_{\pi^\pm} - M_{\pi^0}$ ➛ disconnected diagrams, very noisy
  - ✗ From $e^-$ $e^-$ scattering ➛ far too low energy
  - ✗ From $M_{\Sigma^+} - M_{\Sigma^-}$ ➛ baryon has inferior precision
  - ✓ Take renormalized $\alpha$ 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



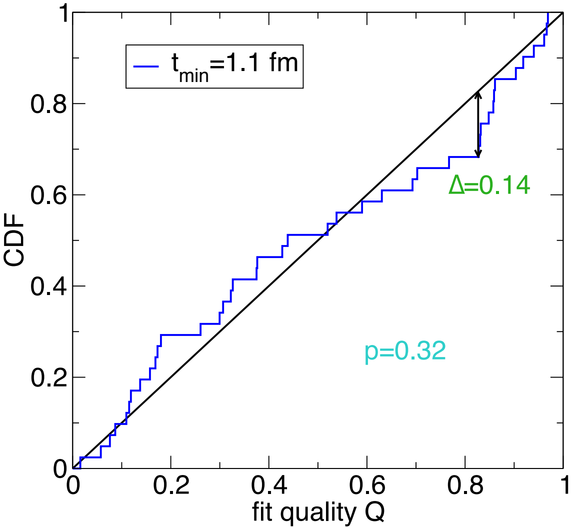
# Plateaux




- 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



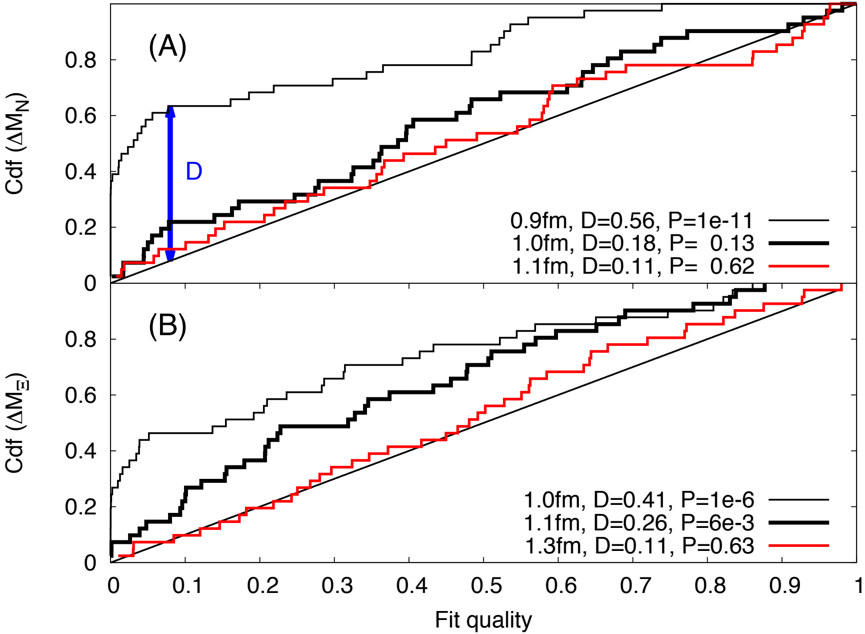

- Need many ensembles
- Plot CDF
- KS test flat distribution

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

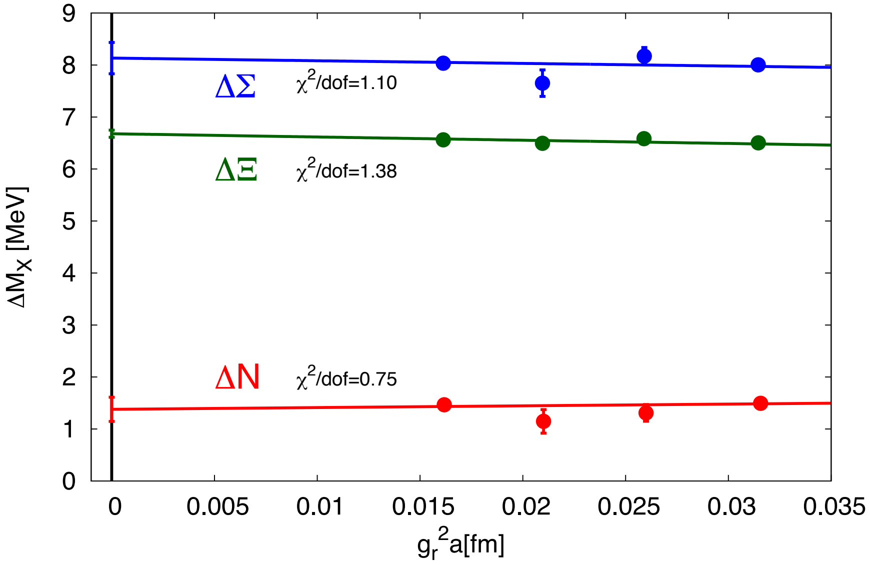
$$p(\Delta(\sqrt{N} + 0.12 + \frac{0.11}{\sqrt{N}}))$$

with

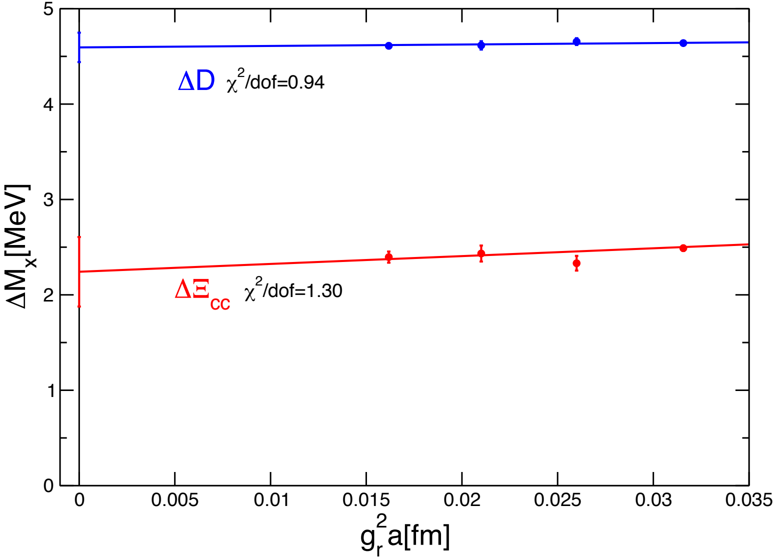
$$p(x) = \sum_j \frac{(-)^{j-1}2}{e^{-2j^2x^3}}$$


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

# 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]

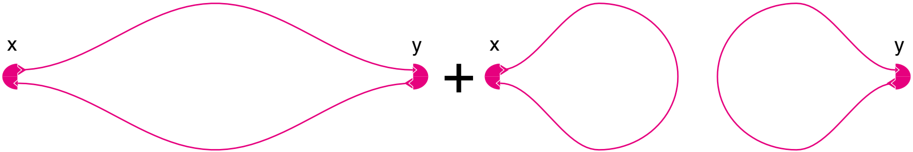
# Scaling


ΔD χ²/dof=0.94
ΔΞcc χ²/dof=1.30
ΔMx[MeV]
g²r 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. $\pi^0$) difficult (disconnected diagrams)




Method:

- Use baryonic splitting $\Sigma^+$-$\Sigma^-$ 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) |
| $\Delta_{\mathrm{CG}}=\Delta N-\Delta\Sigma+\Delta\Xi$ | 0.00(11)(06) | -0.00(13)(05) | 0.00(06)(02) |

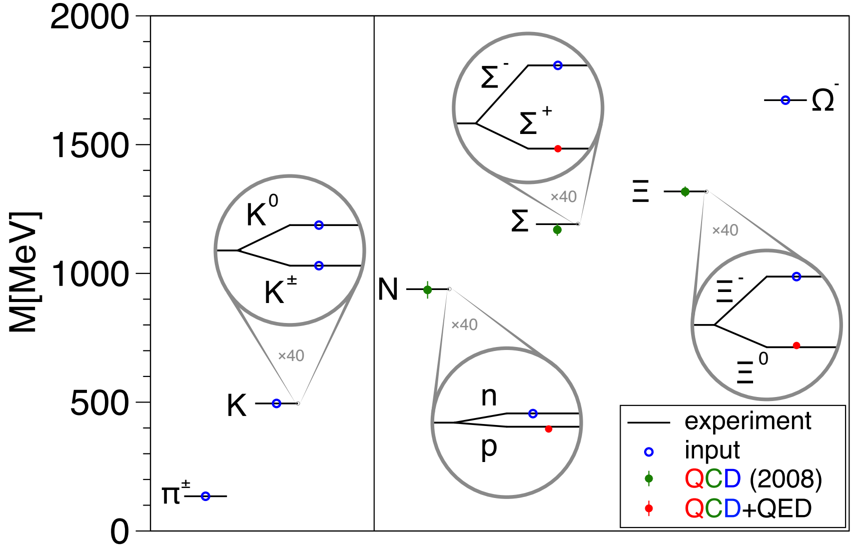
- Quark model relation predicts $\Delta_{\mathrm{CG}}$ to be small

  (Coleman, Glashow, 1961; Zweig 1964)

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

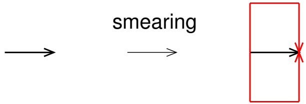
$$\Delta_{\mathrm{CG}} \propto ((m_d - m_u)(m_s - m_u)(m_s - m_d), \alpha(m_s - m_d))$$

# 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

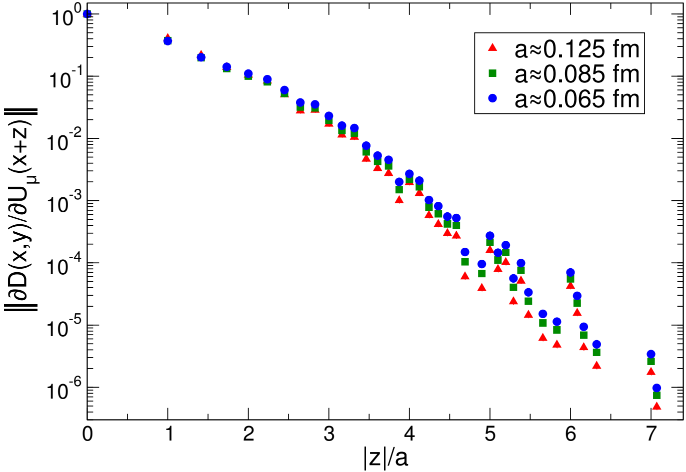



- locality in position space:
  $|D(x,y)| < \text{const}\, e^{-\lambda|x-y|}$ with $\lambda = O(a^{-1})$ for all couplings.
  Our case: $D(x,y) = 0$ as soon as $|x-y| > 1$
  (despite smearing)

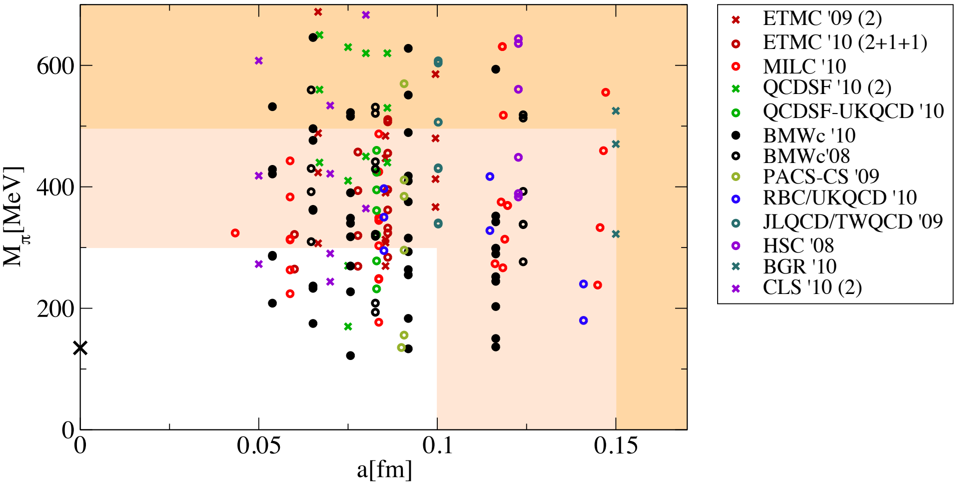
- locality of gauge field coupling:
  $|\delta D(x,y)/\delta A(z)| < \text{const}\, e^{-\lambda|(x+y)/2-z|}$ with $\lambda = O(a^{-1})$ for all couplings.
  Our case: $\delta D(x,x)/\delta A(z) < \text{const}\, e^{-\lambda|x-z|}$ with $\lambda \simeq 2.2a^{-1}$ for $2 \leq |x-z| \leq 6$

# Gauge field coupling locality

6-stout case:



# Landscape $M_\pi$ vs. $a$



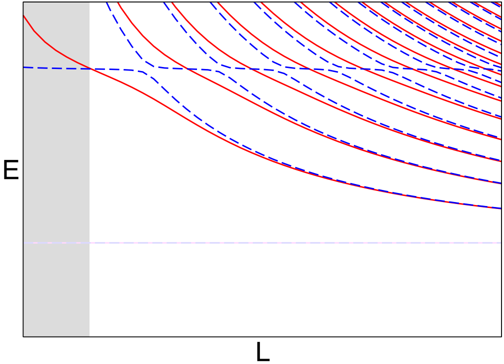
# Finite volume effects in resonances

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

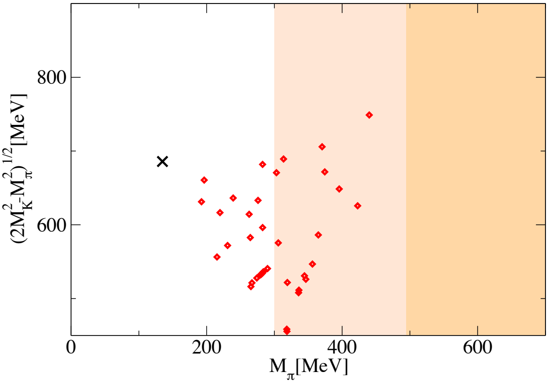



- Treatment as scattering problem

(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:

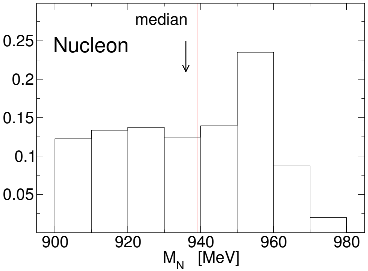
- We account for all the above mentioned effects
- When there are a number of sensible ways to proceed, we take them: Complete analysis for each of
  - 18 fit range combinations
  - ratio/nonratio fits ($r_X$ resp. $M_X$)
  - $O(a)$ and $O(a^2)$ discretization terms
  - NLO $\chi$PT $M_\pi^3$ and Taylor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

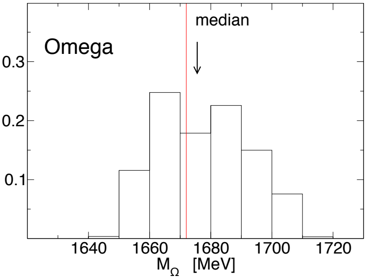
  resulting in 432 (144) predictions for each baryon (vector meson) mass with each 2000 bootstrap samples for each $\Xi$ and $\Omega$ scale setting

# Systematic uncertainties II

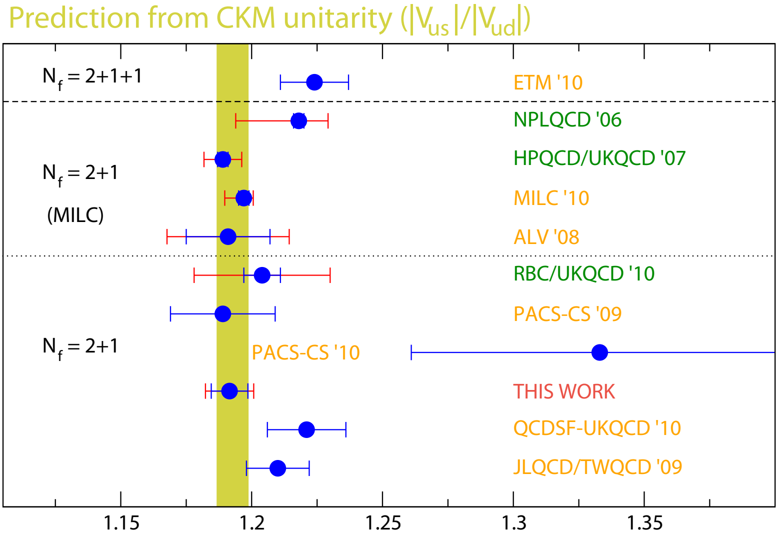
Method (ctd.):

- 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



# $f_K / f_\pi$



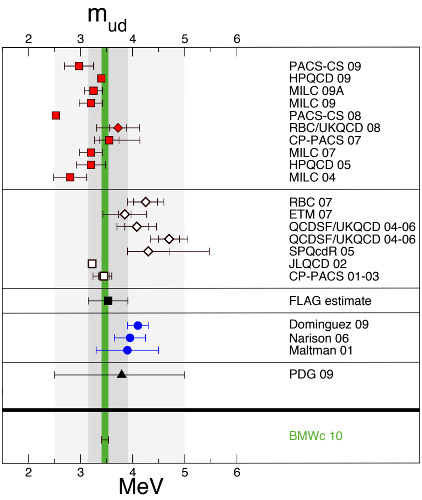
Prediction from CKM unitarity (|V_us|/|V_ud|)
N_f = 2+1+1
ETM '10
NPLQCD '06
HPQCD/UKQCD '07
N_f = 2+1
(MILC)
MILC '10
ALV '08
RBC/UKQCD '10
PACS-CS '09
N_f = 2+1
PACS-CS '10
THIS WORK
QCDSF-UKQCD '10
JLQCD/TWQCD '09
1.15
1.2
1.25
1.3
1.35

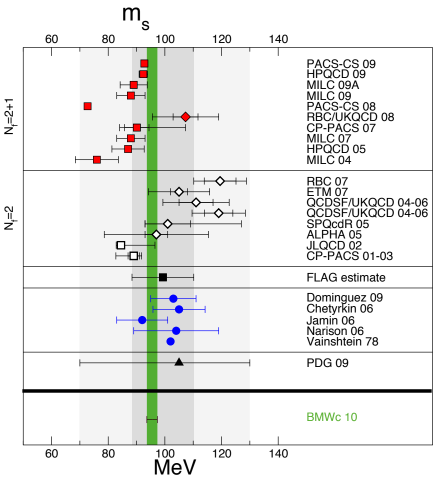
# Individual $m_u$ and $m_d$

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

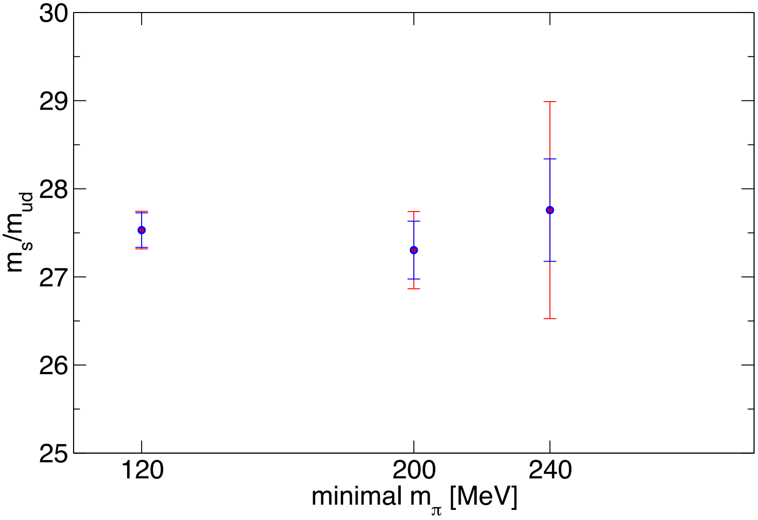
    $Q^2 = \frac{1}{2}\left(\frac{m_s}{m_{ud}}\right)^2 \frac{m_d - m_u}{m_{ud}}$
  - ✓ Transform precise $m_s/m_{ud}$ into $(m_d - m_u)/m_{ud}$
  - We use the conservative $Q = 22.3(8)$ (Leutwyler, 2009)

# 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

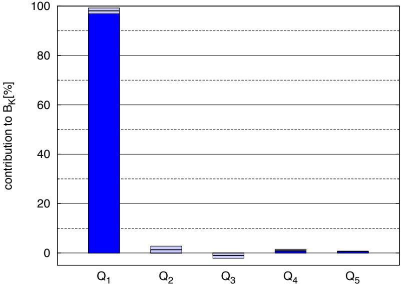

m_s
60
80
100
120
140
N_f=2+1
N_f=2
PACS-CS 09
HPQCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPQCD 05
MILC 04
RBC 07
ETM 07
QCDSF/UKQCD 04-06
QCDSF/UKQCD 04-06
SPQcdR 05
ALPHA 05
JLQCD 02
CP-PACS 01-03
FLAG estimate
Dominguez 09
Chetyrkin 06
Jamin 06
Narison 06
Vainshtein 78
PDG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

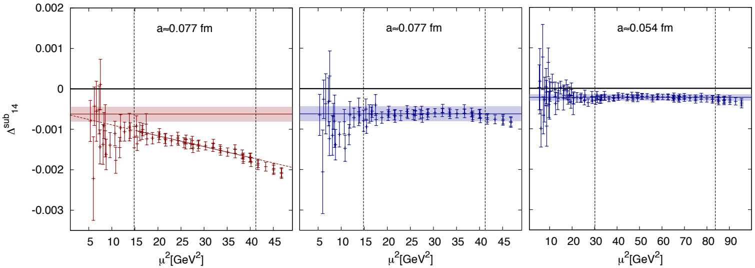
# Chiral cuts



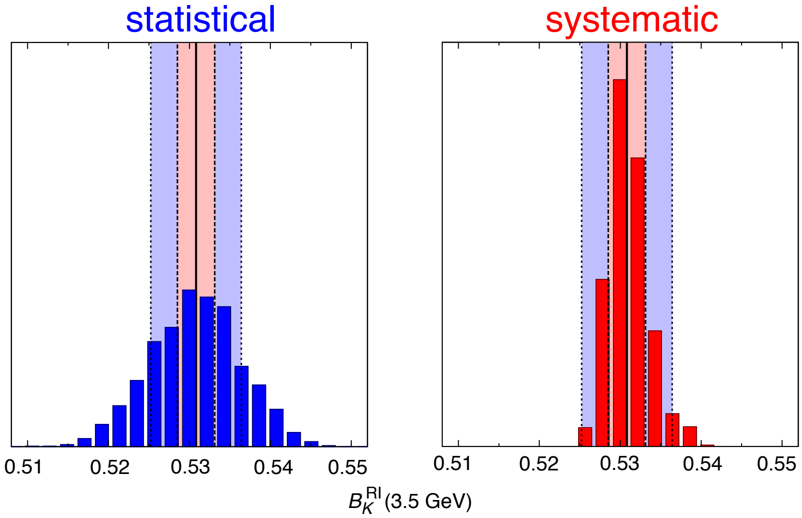
# Unphysical operator mixing

- ☞ $\chi$SB induces mixing with 4 unphysical operators
- ☞ Mixing terms chirally enhanced
- ✓ Small even below physical $m_\pi$
- ✓ Good chirality of our action

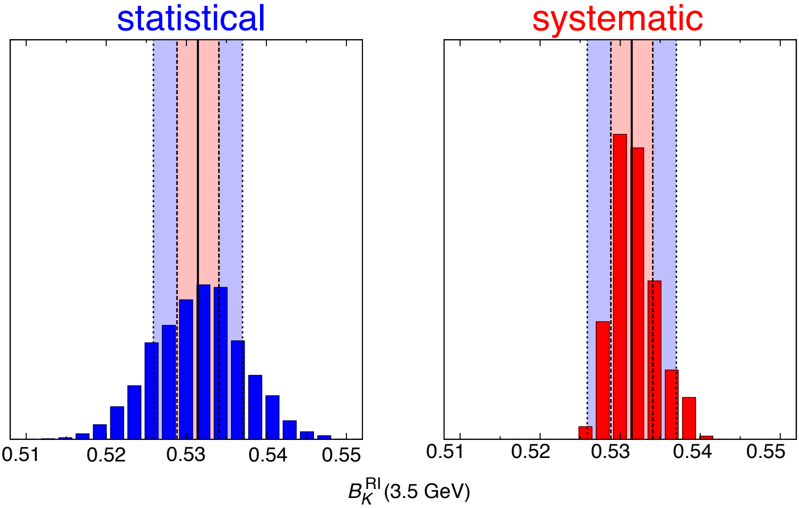


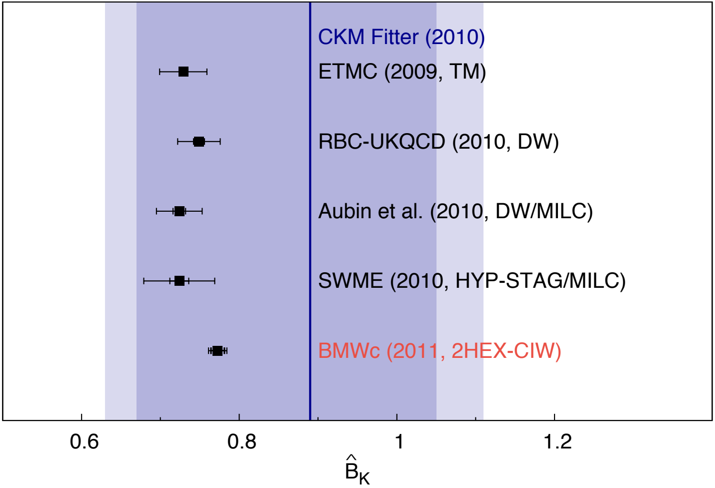
# Errors



# Errors - unit weight

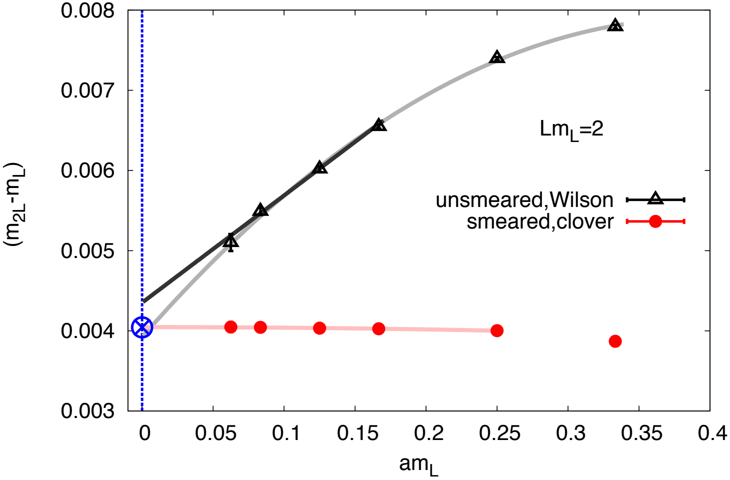


# Comparison




(PLB 705:477,2011)

# 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

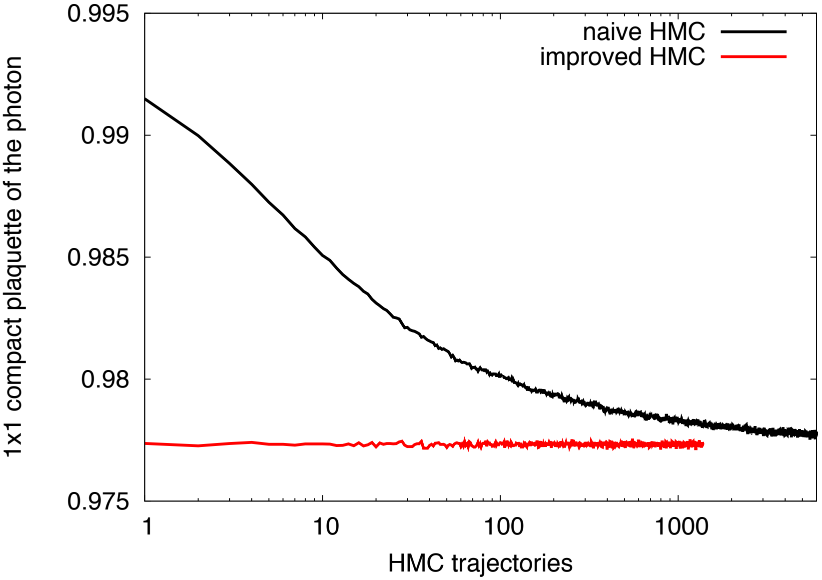
$$\mathcal{H} = \frac{1}{2V_4} \sum_{\mu,k} \left( |\hat{k}|^2 |A_\mu^k|^2 + \frac{|\Pi_\mu^k|^2}{m_k} \right)$$

- Use different masses per momentum

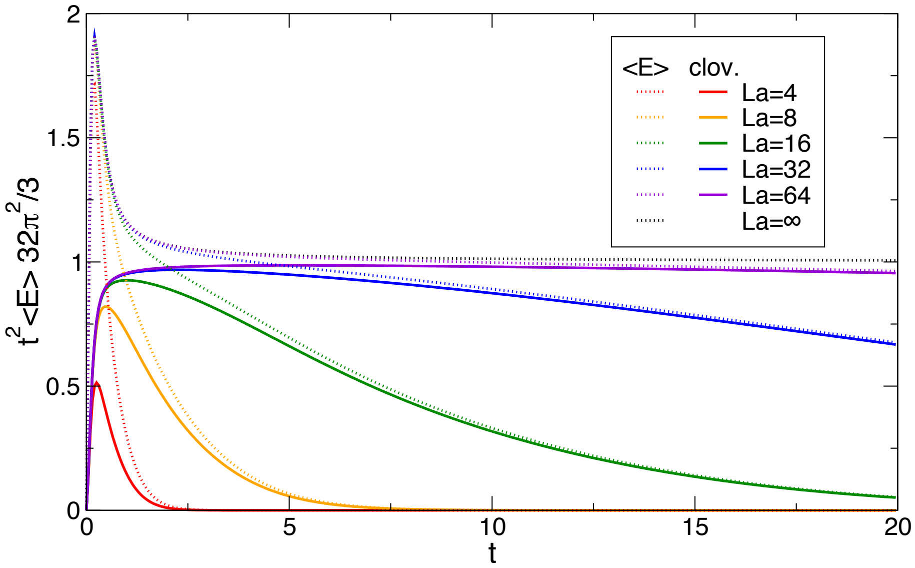
$$m_k = \frac{4|\hat{k}|^2}{\pi^2}$$

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

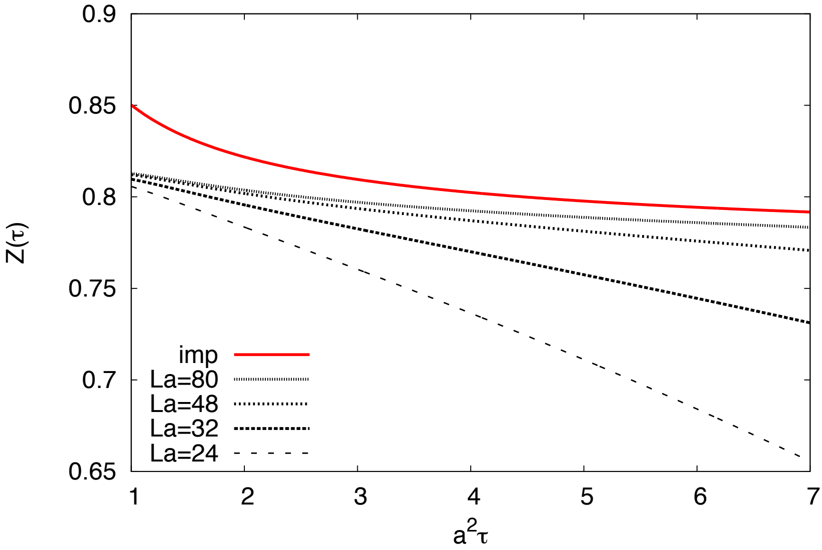
# HMC FOR PHOTON FIELDS



# TREE LEVEL CORRECTION



# EFFECT OF TREE LEVEL CORRECTION



# SCALING IN RENORMALISED COUPLING

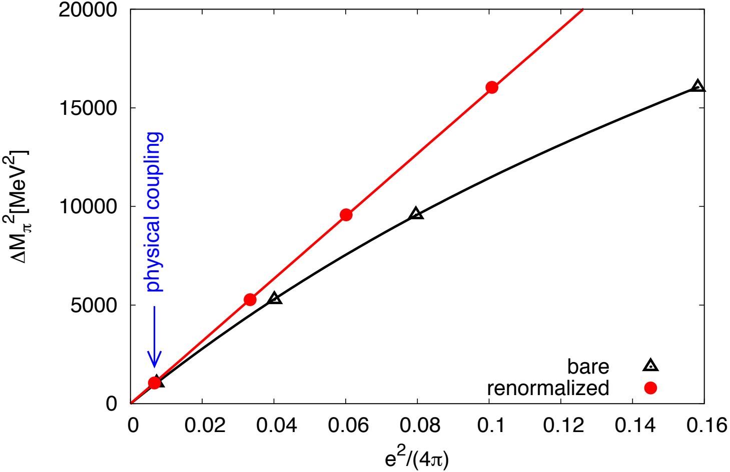
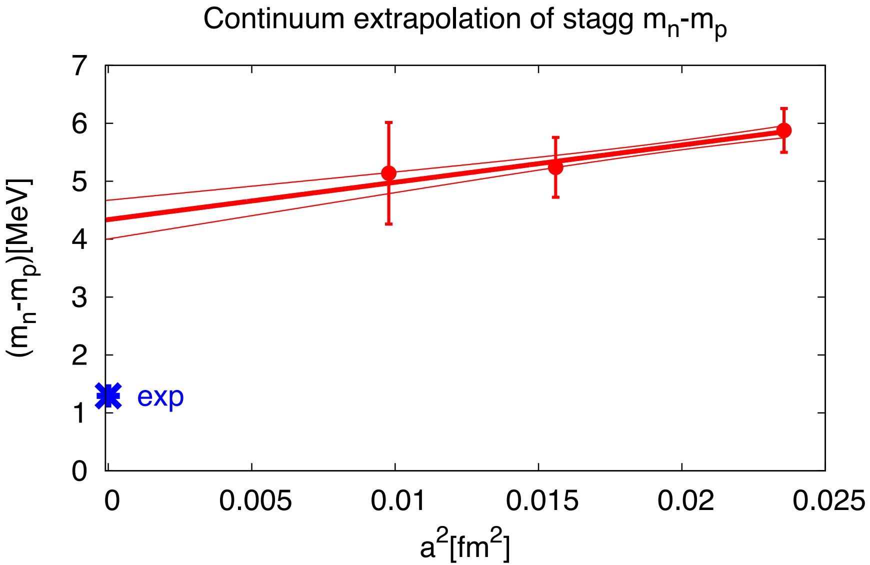



Illustration with precise $\Delta M_\pi^2 = M_{\bar{u}d}^2 - (M_{\bar{u}u}^2 + M_{\bar{d}d}^2)/2$

# DONT DO THIS STAGGERED



# Combining results

How to determine the spread of results?

- Stdev or $1\sigma$ 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 $\Gamma_i$ from unknown pdf $g(\Gamma)$
- Fit model $f(\Gamma|\Theta)$ with parameters $\Theta$
- 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?