The nucleon quark content from lattice QCD

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(Science 322:1224 (2008))

(Science 347: 1452 (2015))

(Phys.Rev.Lett. 116 (2016) no.17, 172001)

Budapest-Marseille-Wuppertal connaboration

How to compute the quark content of the nucleon?

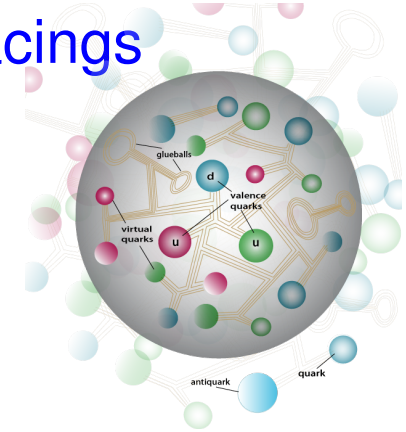
Problem:

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

☞Basic recipie:

- Solve QCD for various quark masses and lattice spacings

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

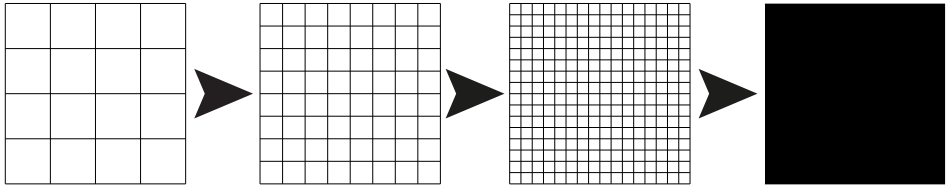


- Define physical point by dimensionless experimental ratios (between e.g. $m_\pi/M_\Omega, m_K/m_\Omega$)
- Extrapolate to the physical point and read off result
- Everywhere else, results are ambiguous!

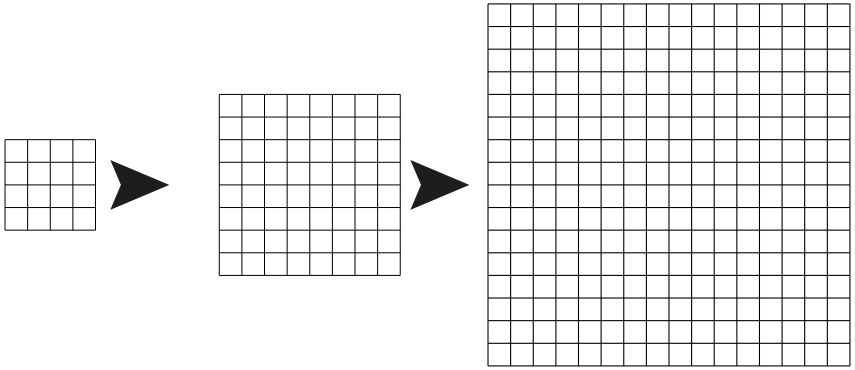
Lattice

Lattice QCD=QCD when

- Cutoff removed (continuum limit)



- Infinite volume limit taken

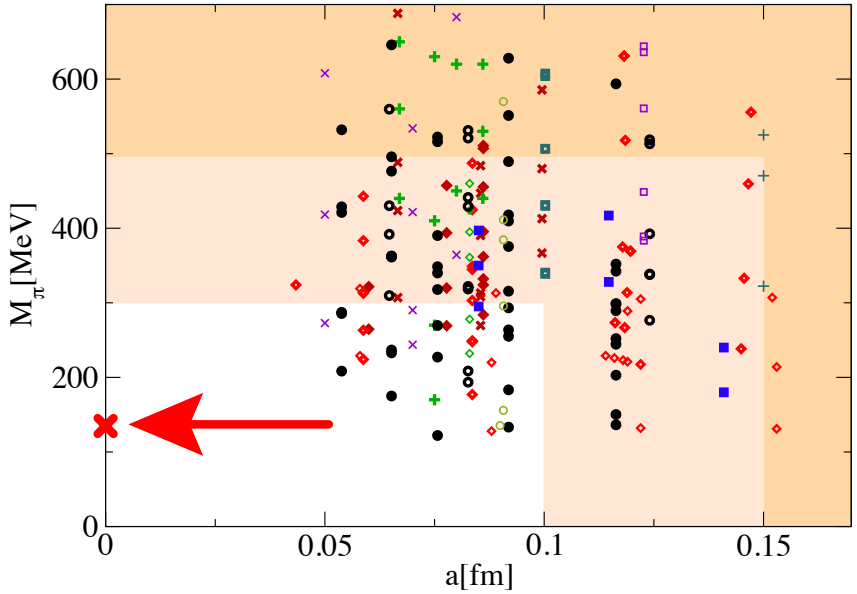


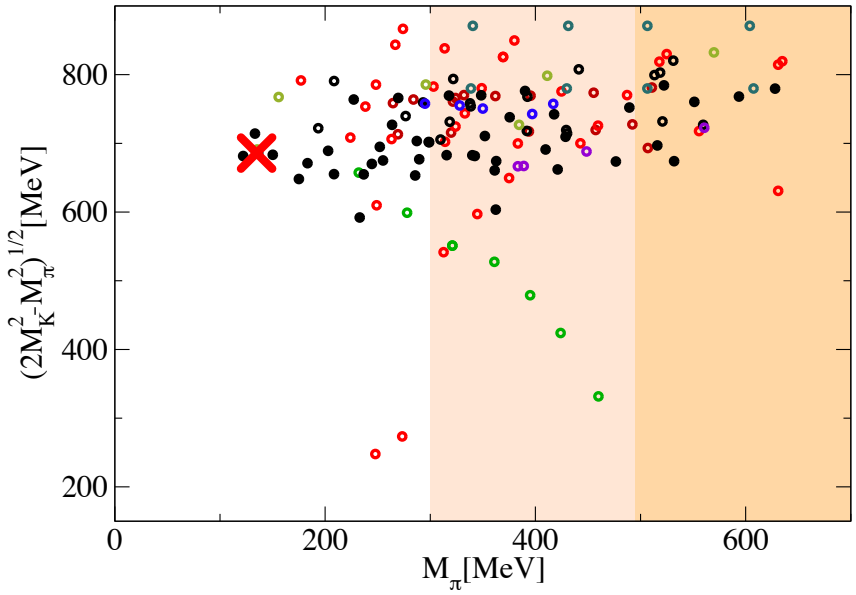
- At physical hadron masses (Especially π)
  - Numerically challenging to reach light quark masses

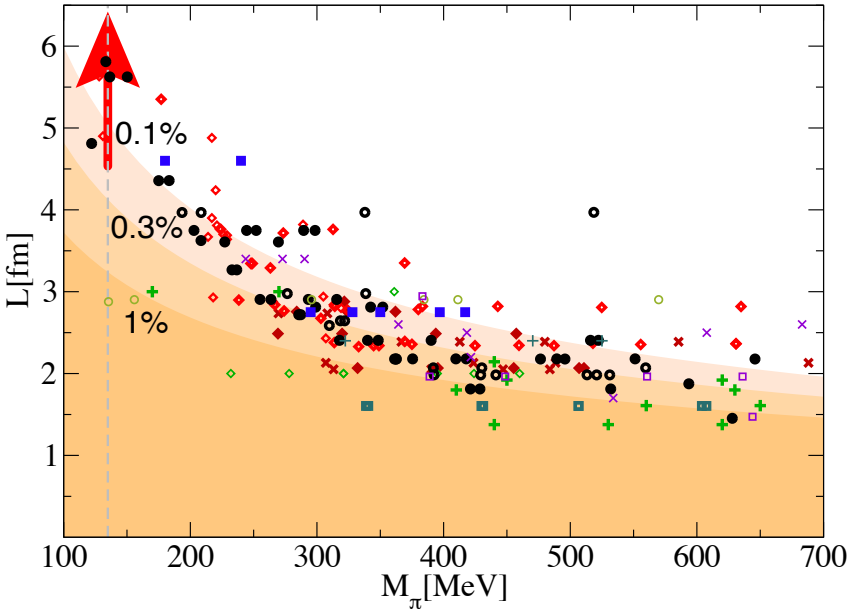
Statistical error from stochastic estimate of the path integral

Extracting a physical prediction

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

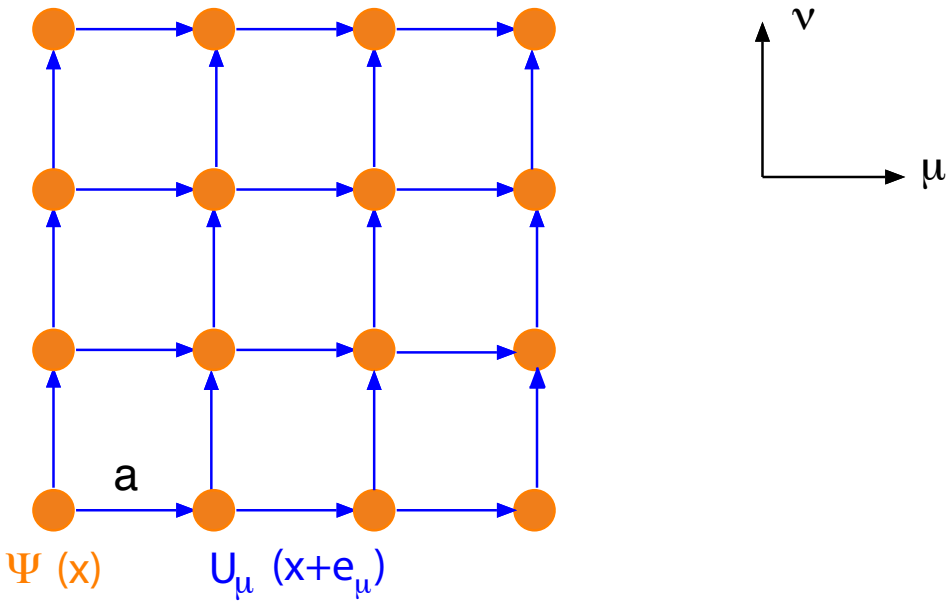






How to solve QCD?

- Wick-rotation: $t \to it$
- UV cutoff: space-time lattice
- Hypercubic, lattice spacing a
- Momentum cutoff $p_\mu < 2\pi/a$
- Continuum theory: $a \to 0$
- Works b/c asymptotic freedom



☞ Anticommuting quark fields $\Psi(x)$ on lattice points

☞ Gluon fields $U_\mu(x) = U(x, x + e_\mu)$ on links

$$U(x,y) = \exp\left(ig \int_x^y dz_\mu \, A_\mu(z)\right) \in SU(3)$$

Path integral

Action of euclidean lattice QCD:

$$S = S_G + S_F$$

where the fermionic part is bilinear in the Grassmann-variables

$$S_F = \bar{\Psi} M \Psi$$

Results from stochastic integration of the path integral:

$$\mathcal{Z} = \int \prod_{x,\mu} [dU_\mu(x)][d\bar{\Psi}(x)][d\Psi(x)] e^{-S_G - S_F}$$
$$= \int \prod_{x,\mu} [dU_\mu(x)] \det(M[U]) e^{-S_G}$$

M is a matrix $\sim 10^9 \times 10^9$

Quark propagators from:

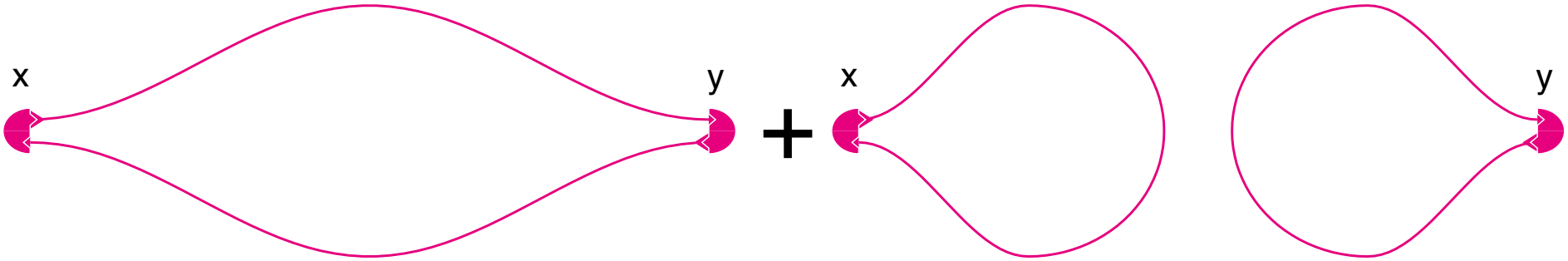
$$\int \prod_{z,\mu} [dU_\mu(z)][d\bar{\Psi}(z)][d\Psi(z)]\Psi_\alpha(x)\bar{\Psi}_\beta(y)e^{-S_G-S_F} =$$

$$\int \prod_{z,\mu} [dU_\mu(z)]M^{-1}_{x,\alpha;y,\beta}[U]\det(M[U])e^{-S_G}$$

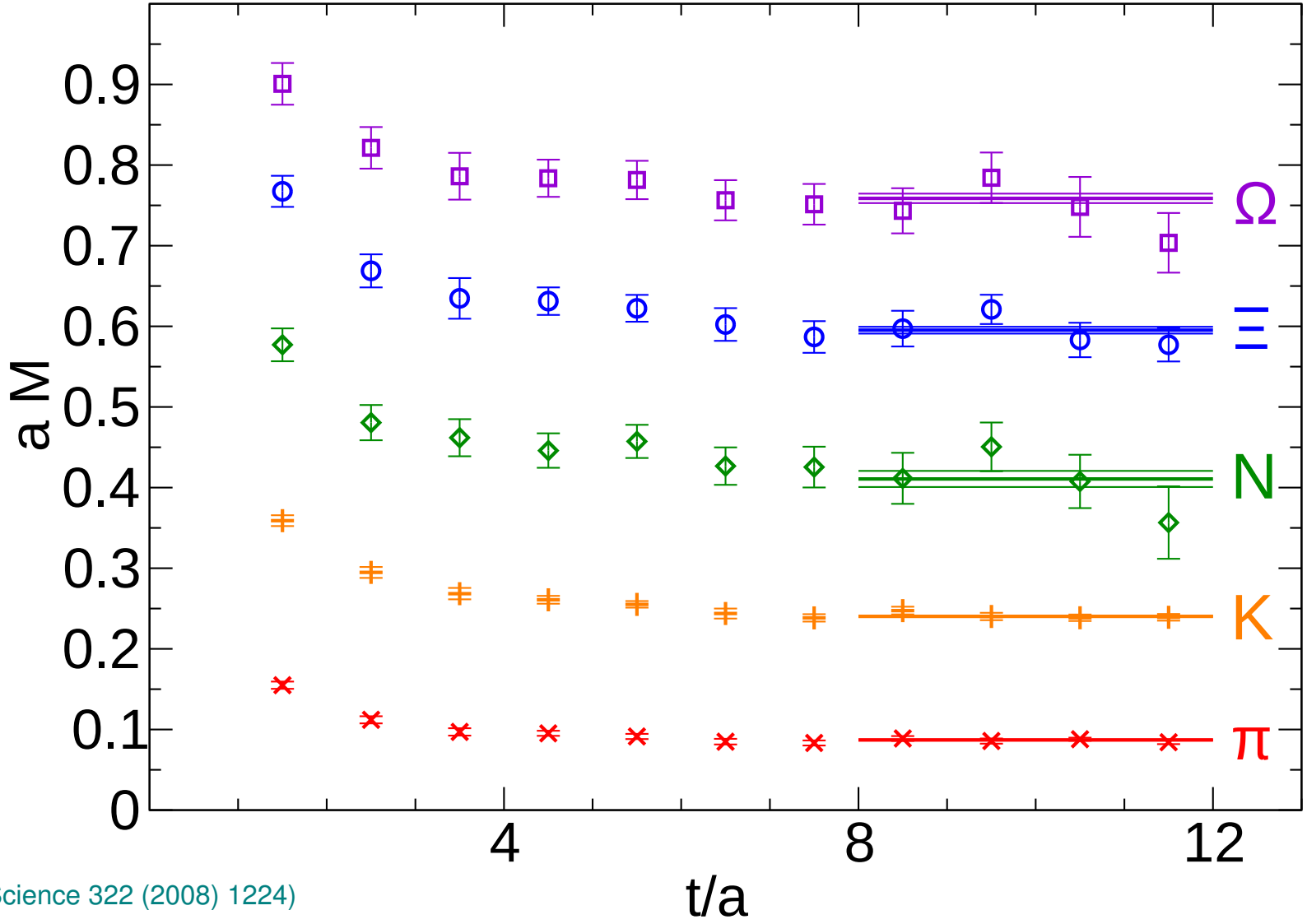
Hadron propagators:

$$\langle 0|T((\bar{\Psi}\Psi)_y(\bar{\Psi}\Psi)_x)|0\rangle = \frac{1}{\mathcal{Z}}\int DUe^{-S_G}\det(M[U])\times$$

$$\left(\left(\mathrm{Tr}\left(M^{-1}_{x,y}(U)M^{-1}_{y,x}(U)\right) + \mathrm{Tr}\left(M^{-1}_{x,x}(U)\right)\left(M^{-1}_{y,y}(U)\right)\right) \right)$$

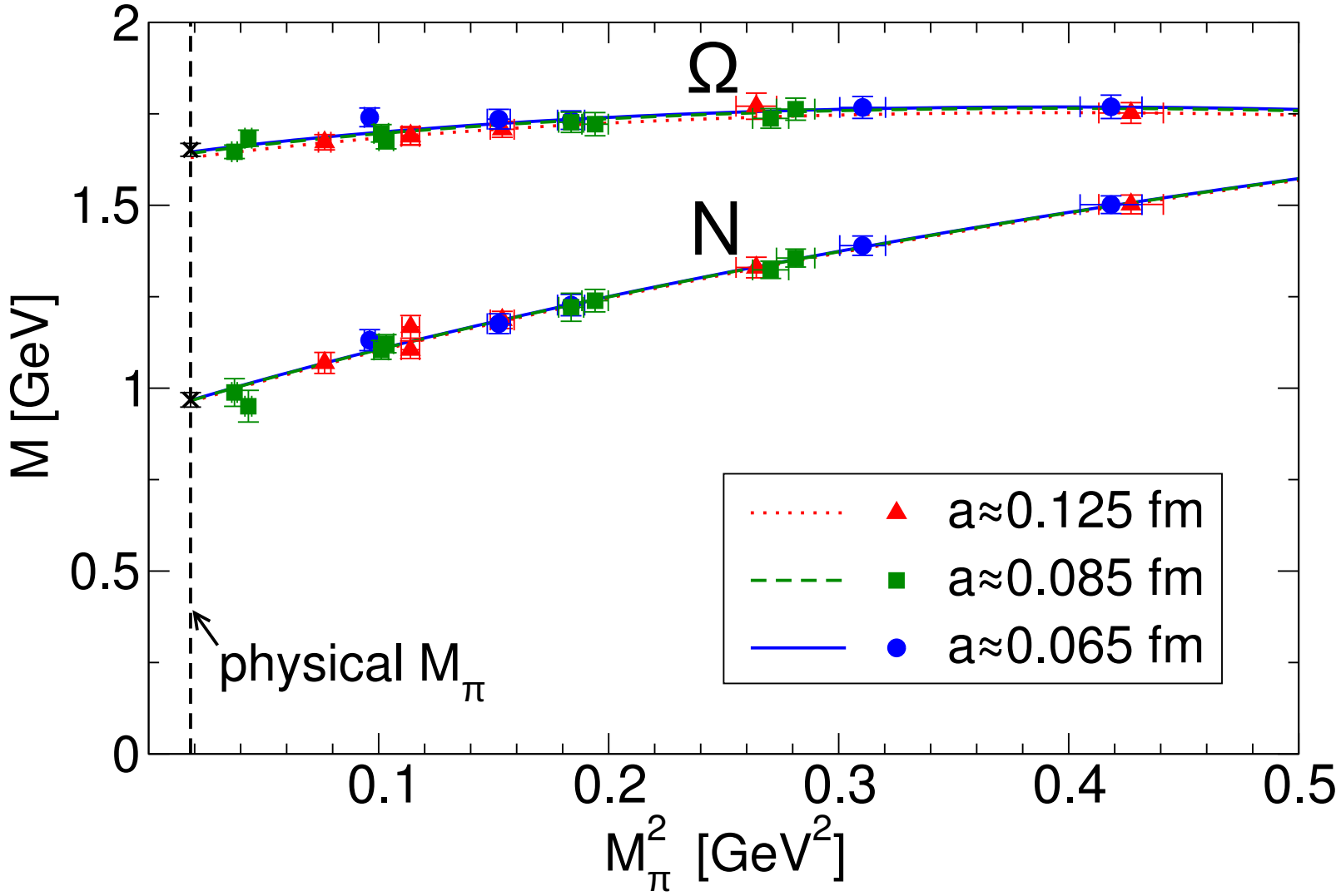


Mass plateaus and fits

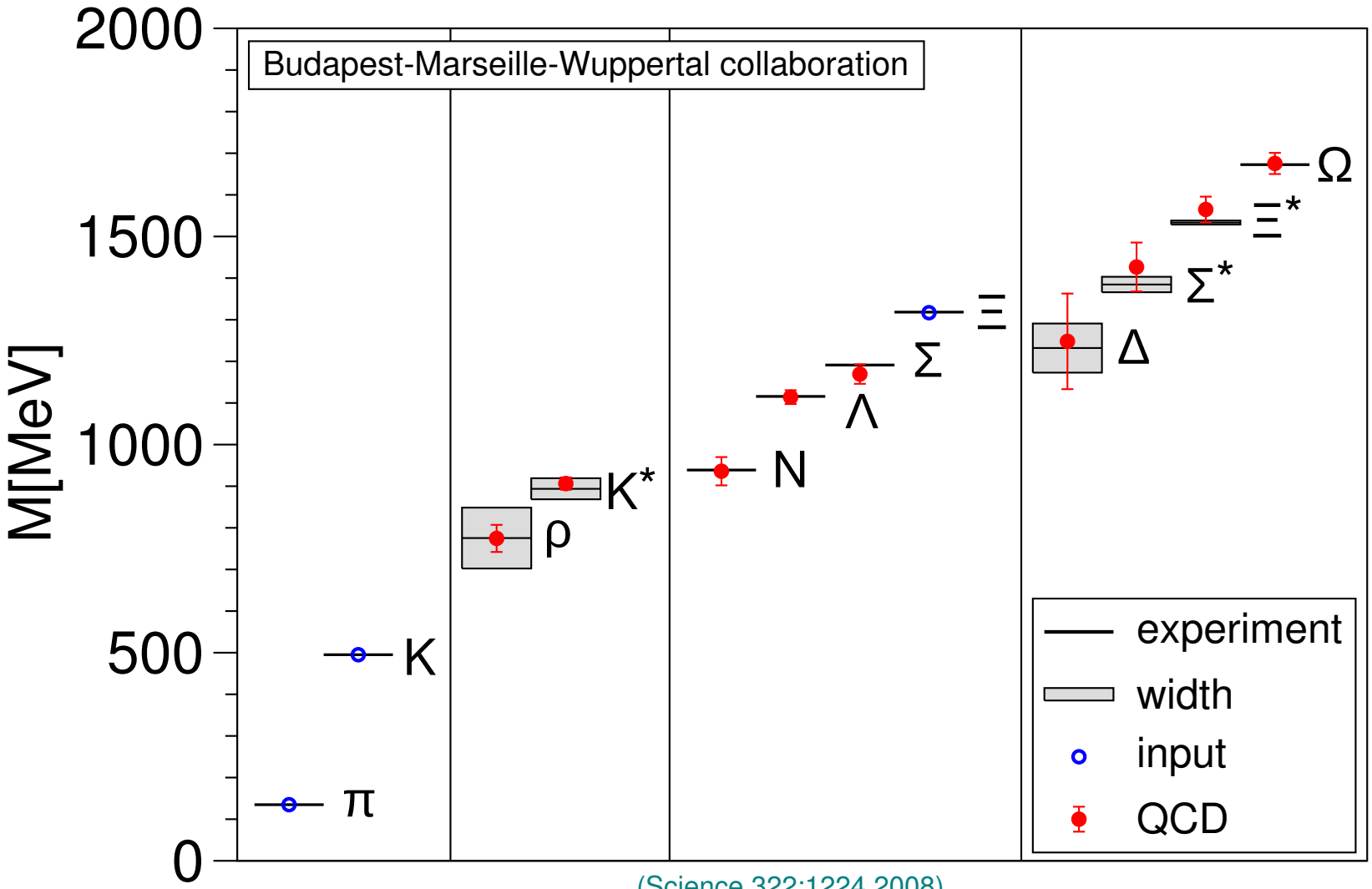


(BMWc, Science 322 (2008) 1224)

Chiral continuum fit



The light hadron spectrum

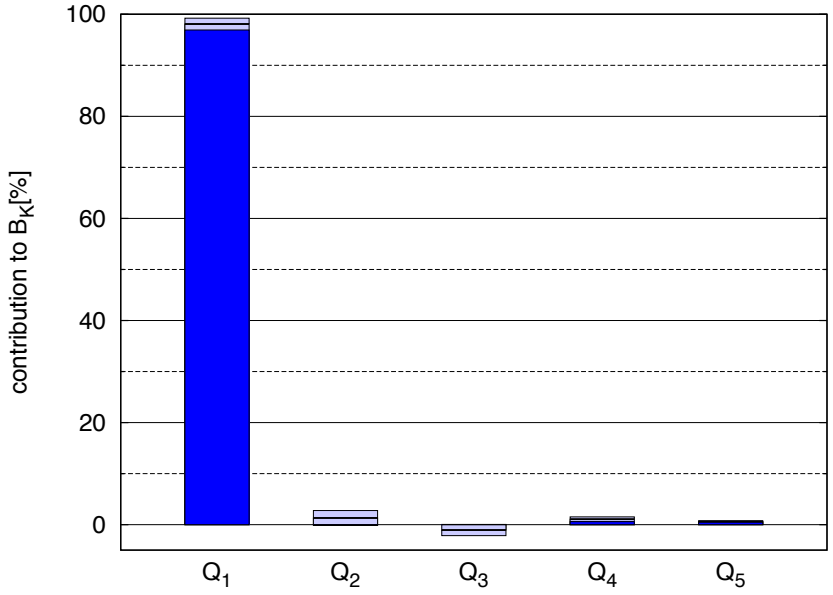


(Science 322:1224,2008)

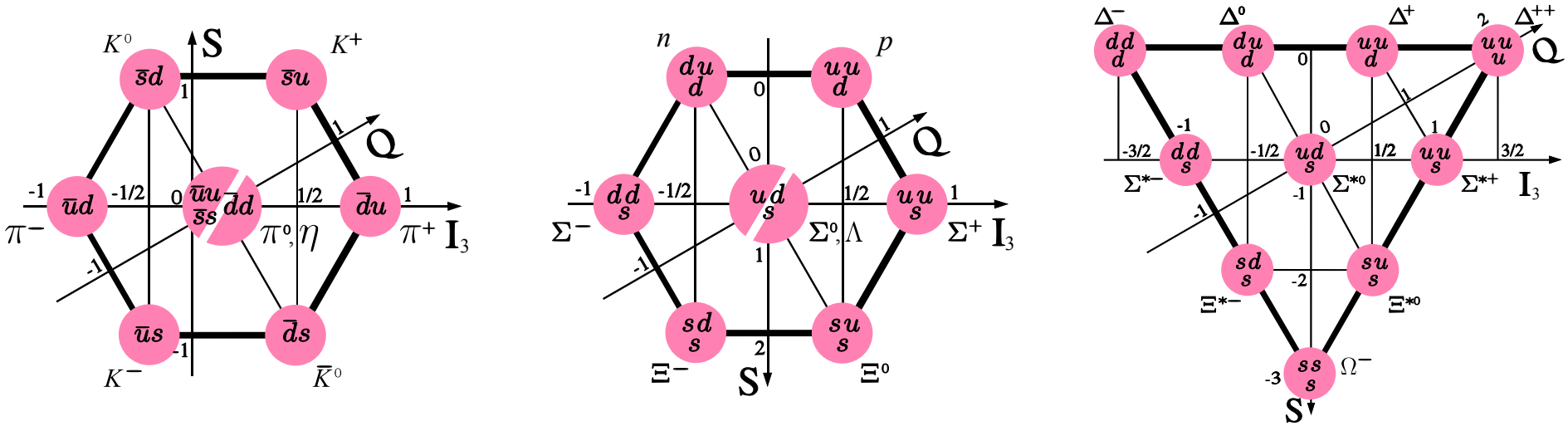
Extracting reliable results

How to obtain useful, reliable results:

- ☞ Fundamentally correct, efficient lattice discretization
  - ✓ "Smeared clover" action (Capitani, Dürr, C.H., 2006)
  - ✓ Dynamical fermions: $2 \times m_{ud} = \frac{m_u + m_d}{2}$ and m_s (2+1)
    More recent: m_u, m_d ,m_s and m_c (4×1)
  - ✓ Excellent chiral properties
- ☞ Full control over systematic errors
  - ✓ Continuum limit
  - ✓ Infinite volume
  - ✓ Physical point, . . .
- ☞ Balance all sources of error
  - ✓ Minimize total error
  - ✓ No single error should dominate



Isospin splitting

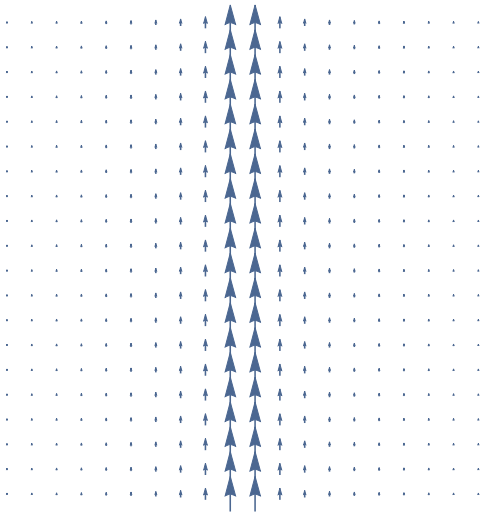


- Two sources of isospin breaking:
  - QCD: $\sim \frac{m_d - m_u}{\Lambda_{QCD}} \sim 1\%$
  - QED: $\sim \alpha(Q_u - Q_d)^2 \sim 1\%$
- On the lattice:
  - Include nondegenerate light quarks $m_u \neq m_d$
  - Include QED

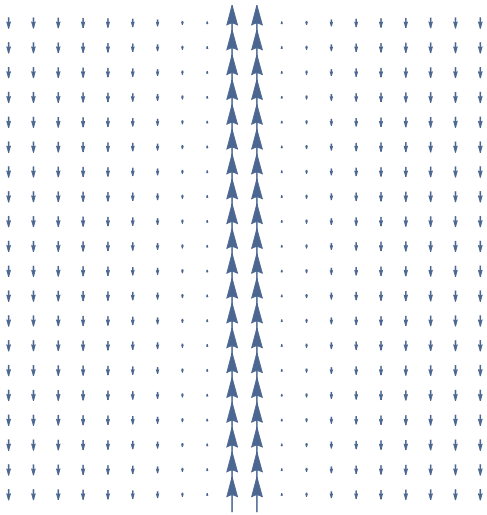
Challenges of QED simulations

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

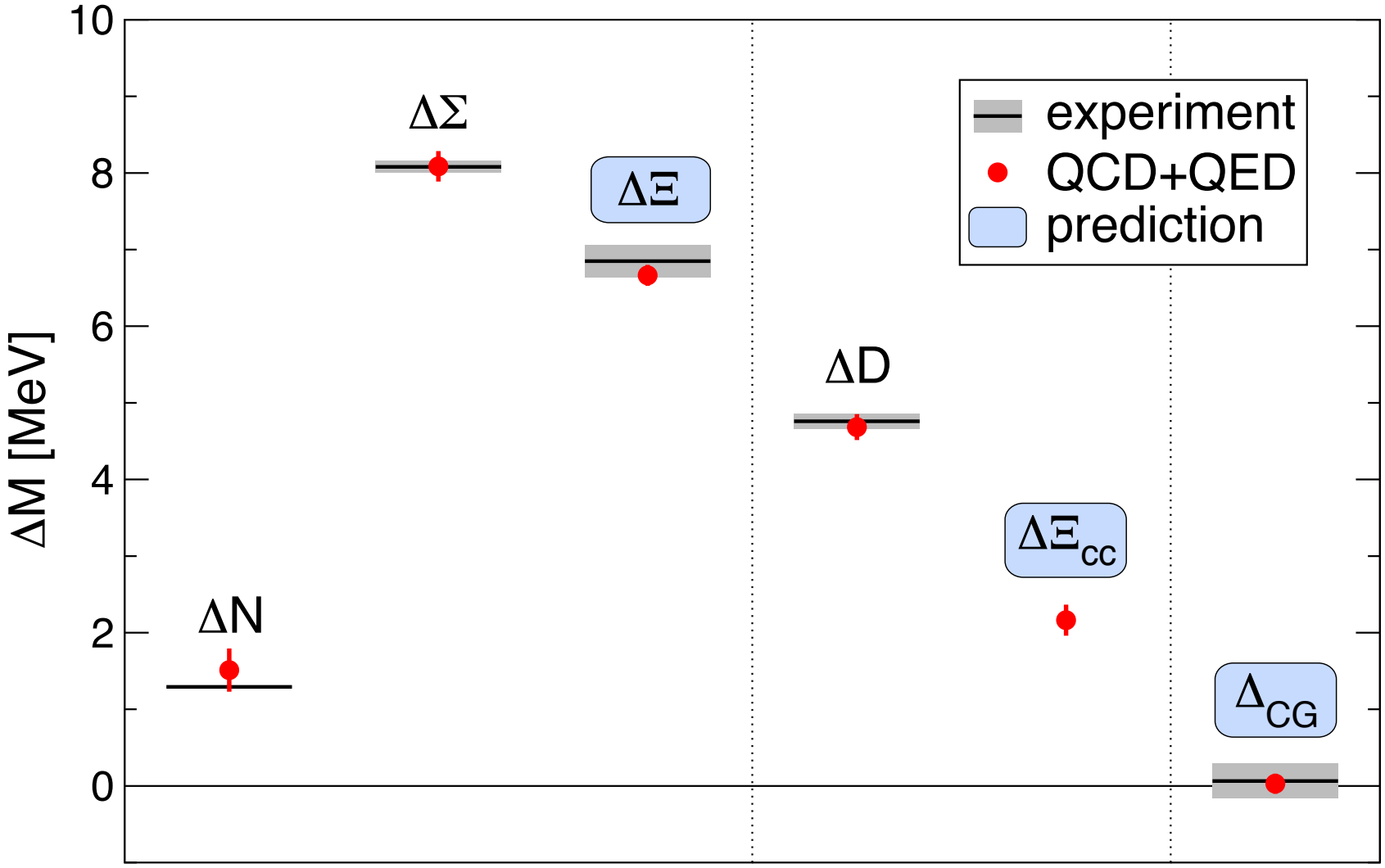
Zero mode of gauge potential unconstrained by action



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



Isospin splitting



(BMWc 2014)

Isospin splittings numerical values

	splitting [MeV]	QCD [MeV]	QED [MeV]
ΔN=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)
$\Delta_{\rm CG}=\Delta N-\Delta\Sigma+\Delta\Xi$	0.00(11)(06)	-0.00(13)(05)	0.00(06)(02)

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

(Coleman, Glashow, 1961; Zweig 1964)

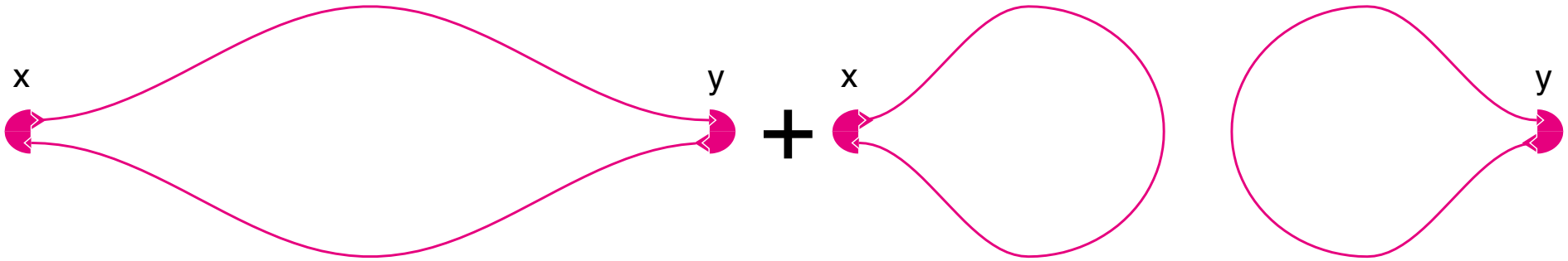
$$\Delta_{\rm CG} = M(udd) + M(uus) + M(dss) - M(uud) - M(dds) - M(uss)$$

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

Disentangling contributions

Problem:

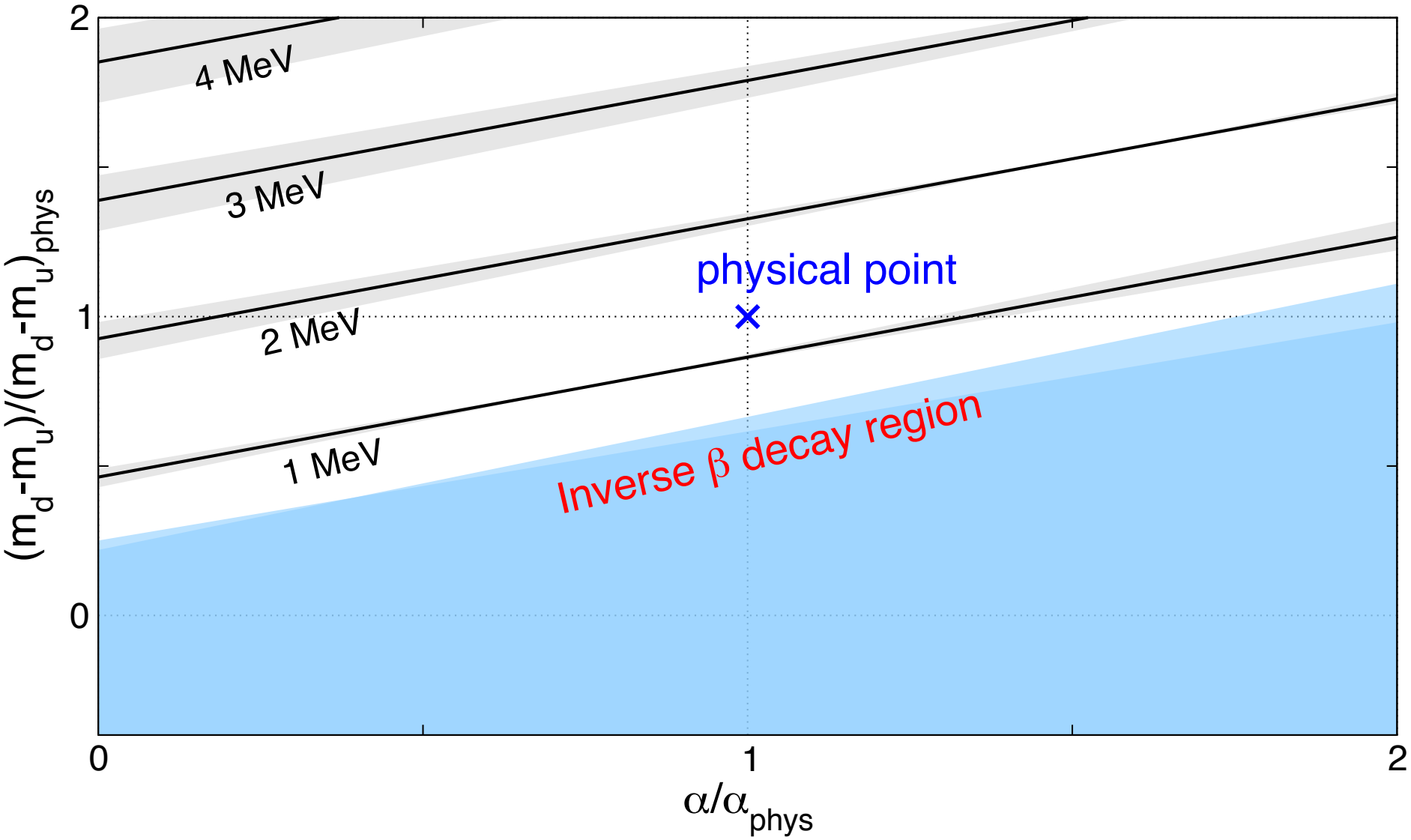
- Disentangle QCD and QED contributions
  - Not unique, $O(\alpha^2)$ ambiguities
- Flavor singlet (e.g. π^0) difficult (disconnected diagrams)



Method:

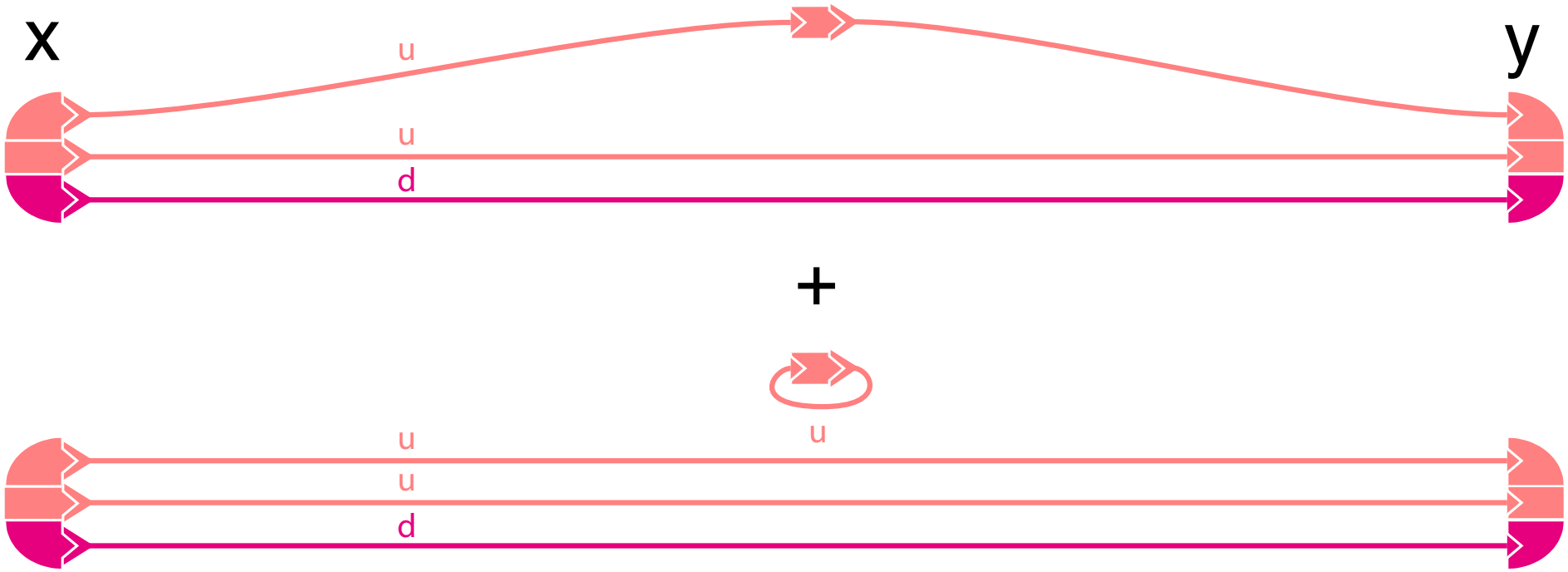
- Use baryonic splitting Σ^+-Σ^- purely QCD
  - Only physical particles
  - Exactly correct for pointlike particle
  - Corrections below the statistical error

Nucleon splitting QCD and QED parts



Nucleon quark content

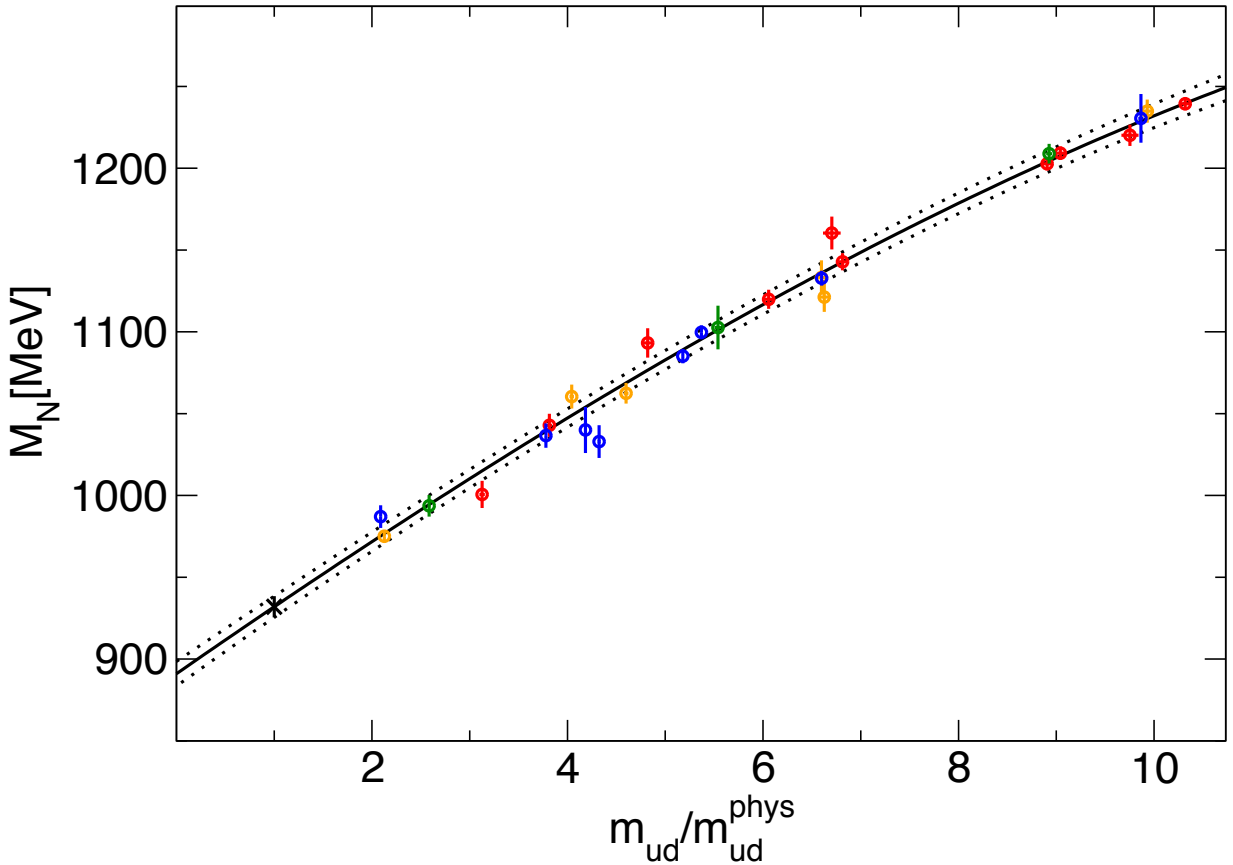
Compute matrix element $m_q \langle N|\bar{q}q|N\rangle$ directly



Or via Feynman-Hellman theorem

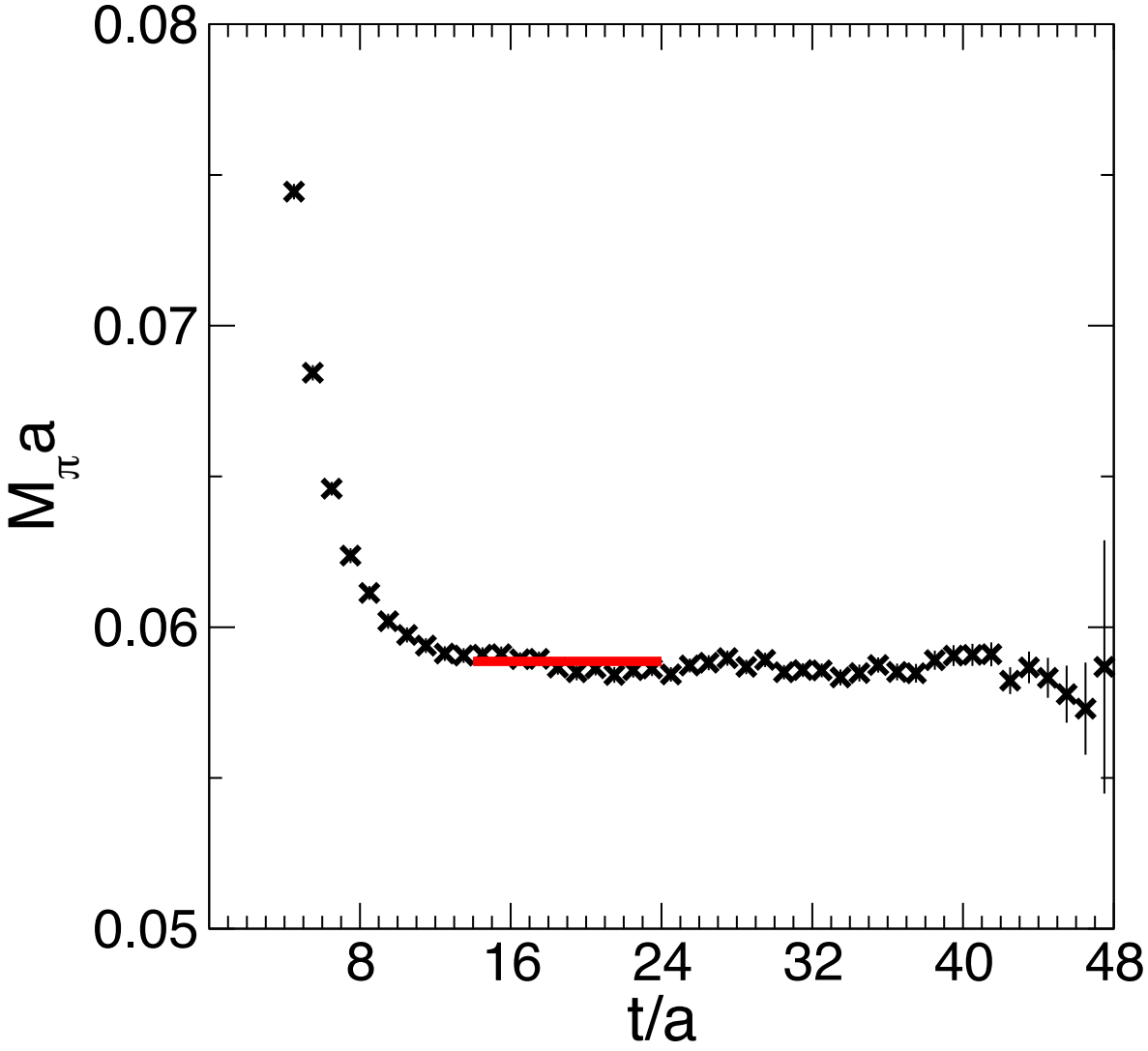
$$\langle N|\bar{q}q|N\rangle = \left.\frac{\partial M_N}{\partial m_q}\right|_{m_q^{\text{phys}}}$$

FH method



- ✓ Simple 2-pt function
- ✓ No disconnected diagrams
- ✓ Easier renormalization
- ☞ Needs accurate slope at physical point

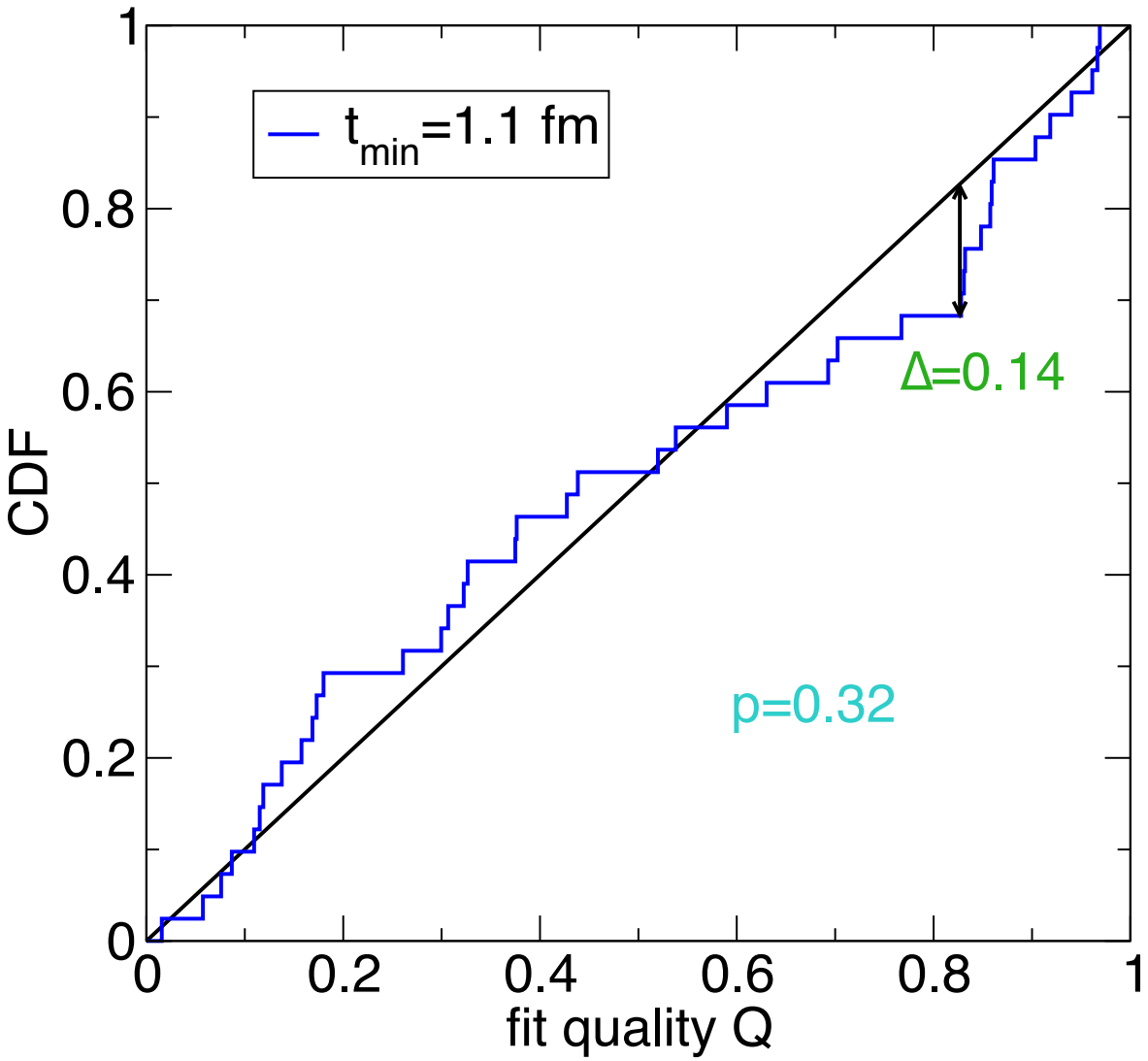
Elimination of excited states



- 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



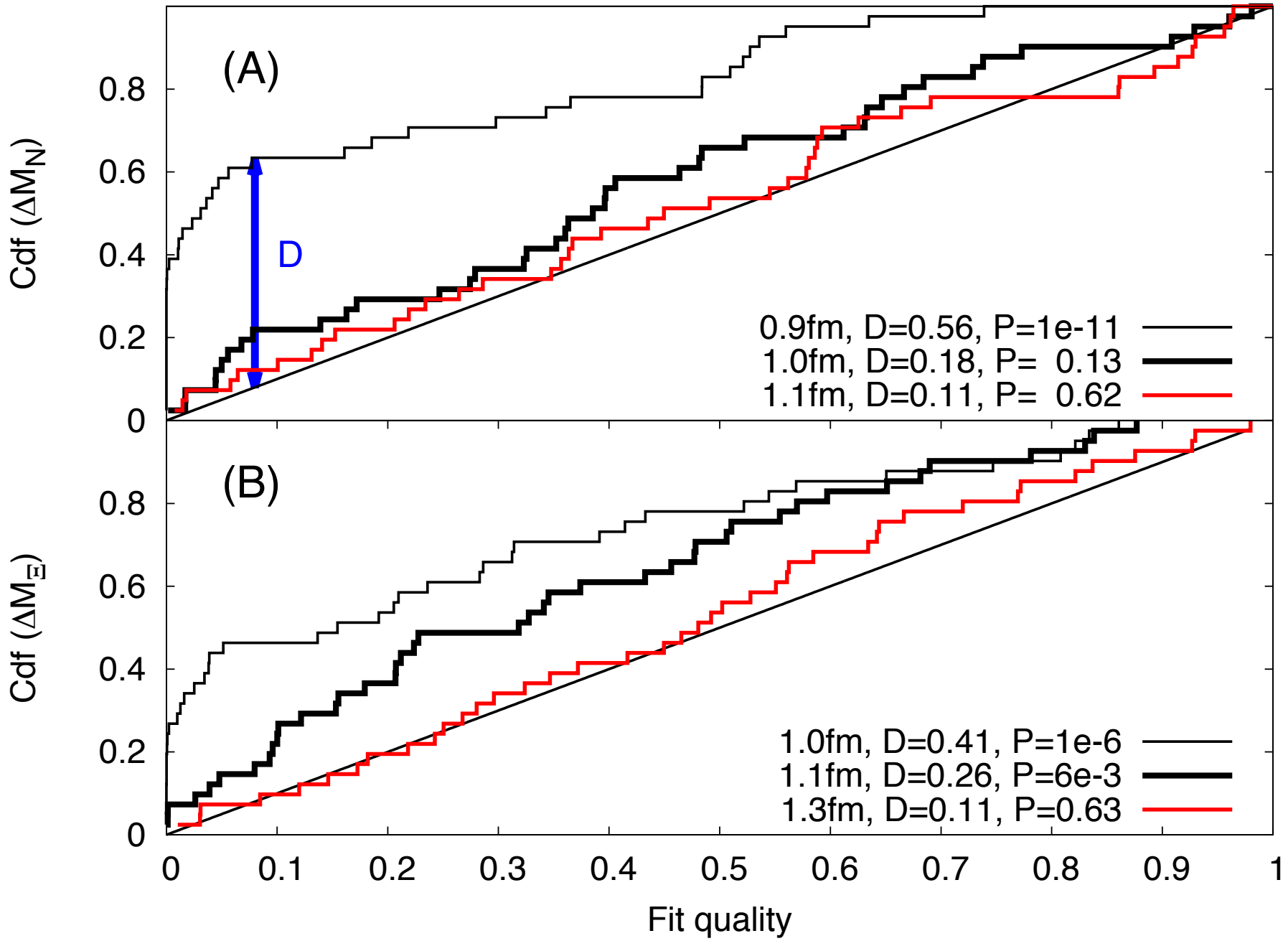
- Need many ensembles
- Plot CDF
- KS test flat distribution

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

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

with

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


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

Analysis strategy

Problem:

- Determine $m_q = m_{ud}, m_s$ dependence of M_N at physical point

Method:

- Determine physical value of m_{ud}, m_s
  - Fit $m_q(M_\pi, M_K, M_{\Omega/N})$ to physical M_π, M_K and $M_{\Omega/N}$
- Determine physical value of $m_q \frac{\partial M_N}{\partial m_q}$
  - Fit $M_N(m_{ud}, m_s)$ to previously determined physical m_{ud} and m_s
- Perform infinite volume and continuum extrapolation
- One global, fully correlated fit
- Estimate systematic error

Quark mass dependence

Problem:

- To define physical quark masses, we need a renormalization scheme

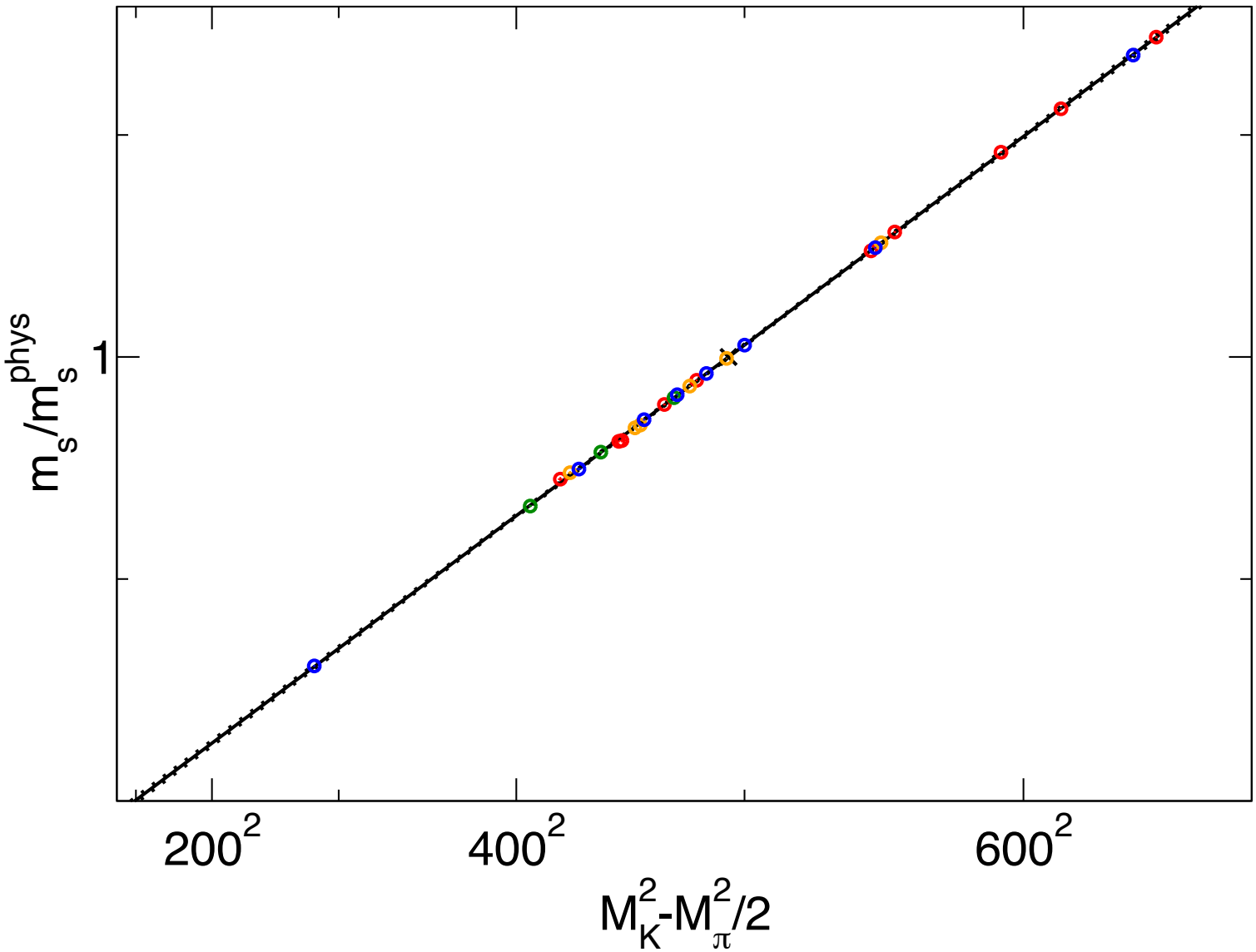
Method:

- Simplest choice on the lattice: $m_s^{\text{phys}} = 1$
  - Equivalent to parameterization

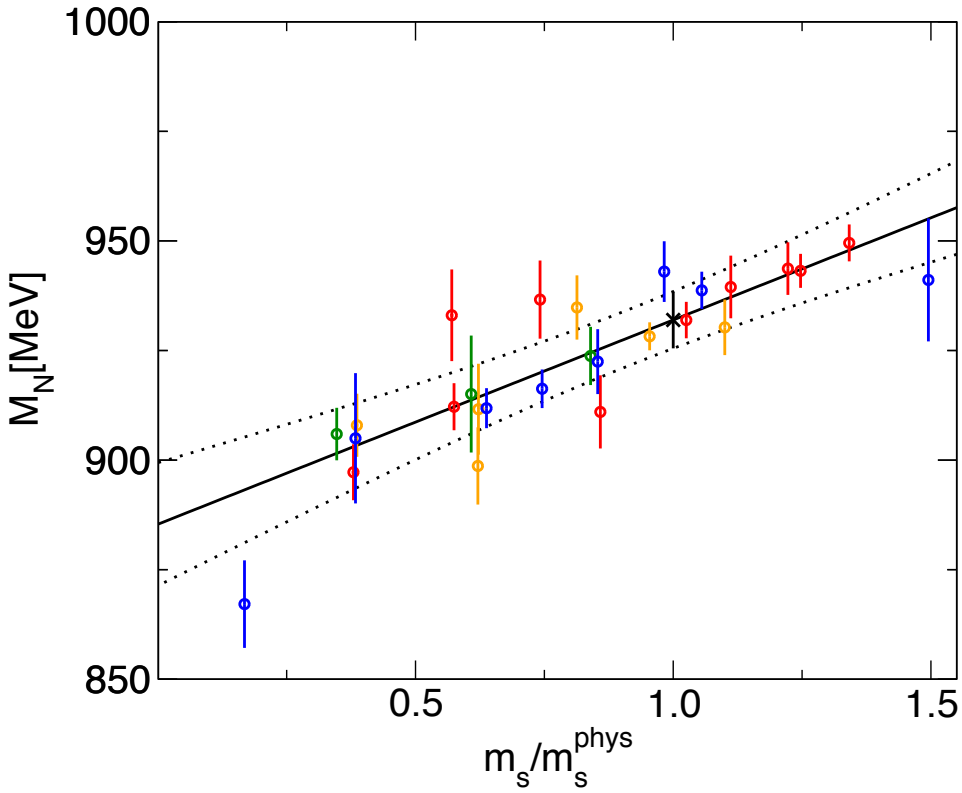
$$c_q \left(\frac{am_q}{aZ_s(\beta)} - m_q^{\text{phys}} \right) \to \tilde{c}_q \left(\frac{am_q}{a\tilde{m}_q^{\text{phys}}(\beta)} - 1 \right)$$

  - Renormalization constants can be computed on the fly
  - Crosscheck with Z_s where available

Quark mass dependence

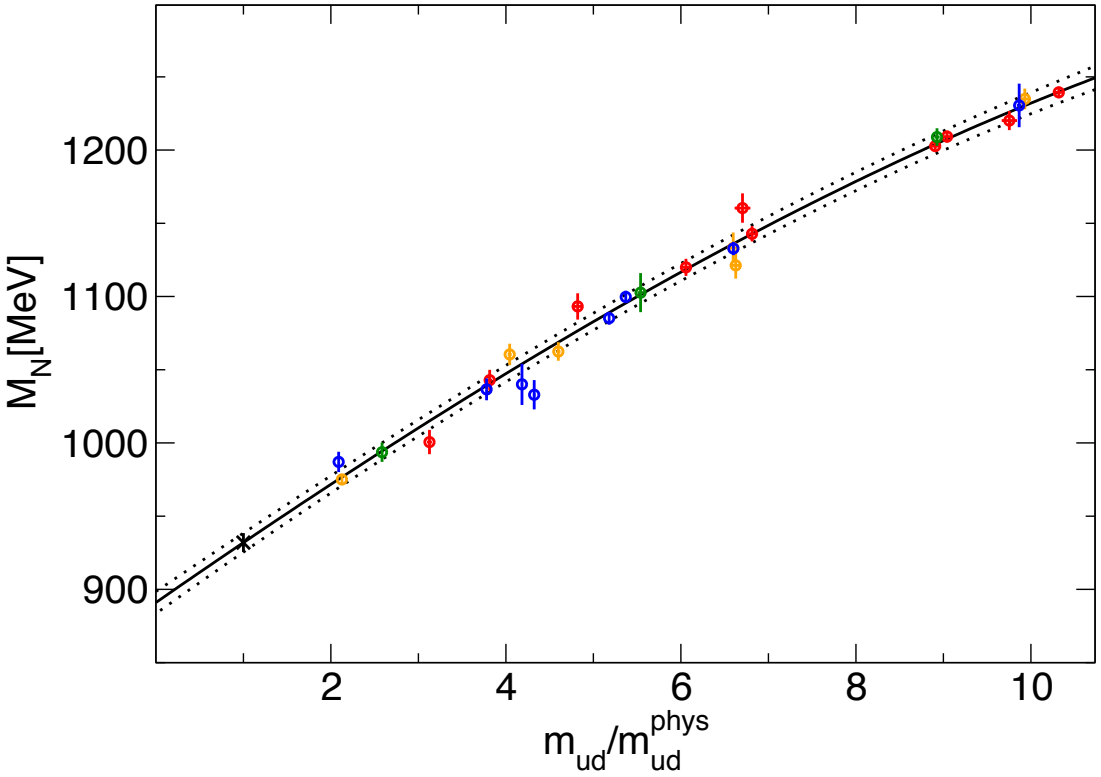


Nucleon fit



- Various Polynomial, Padé and χPT ansätze
- Spread into systematic error

Nucleon fit



- Various Polynomial, Padé and χPT ansätze
- Spread into systematic error

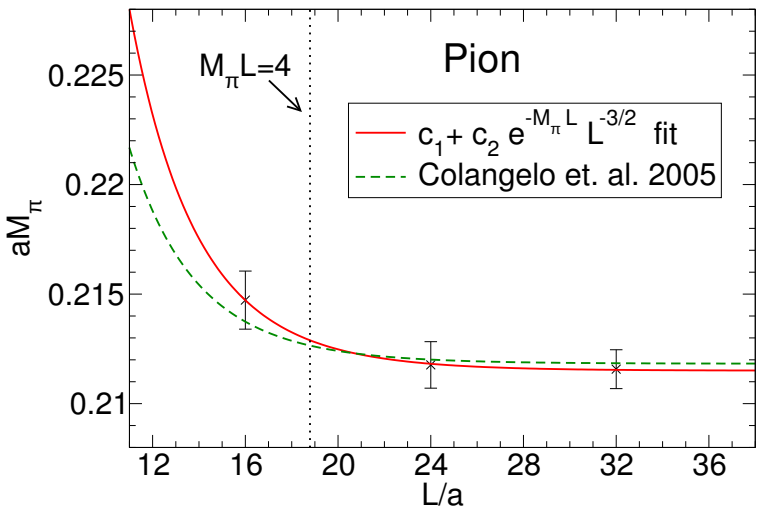
Finite volume effects from virtual pions

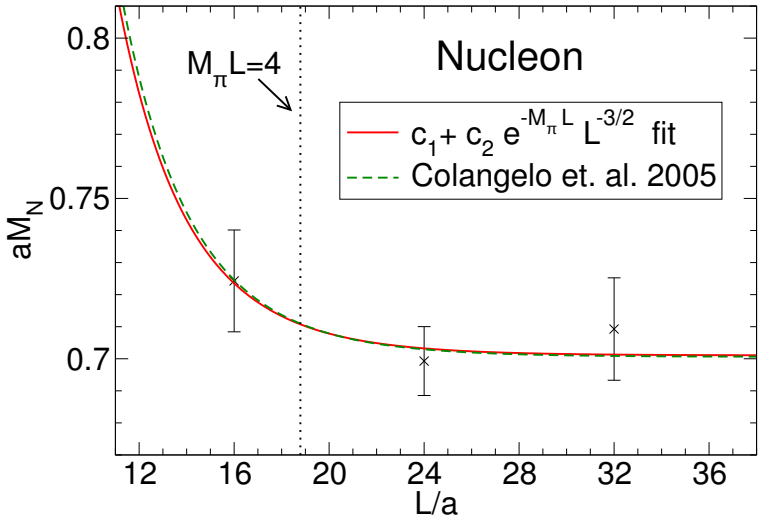
Goal:

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

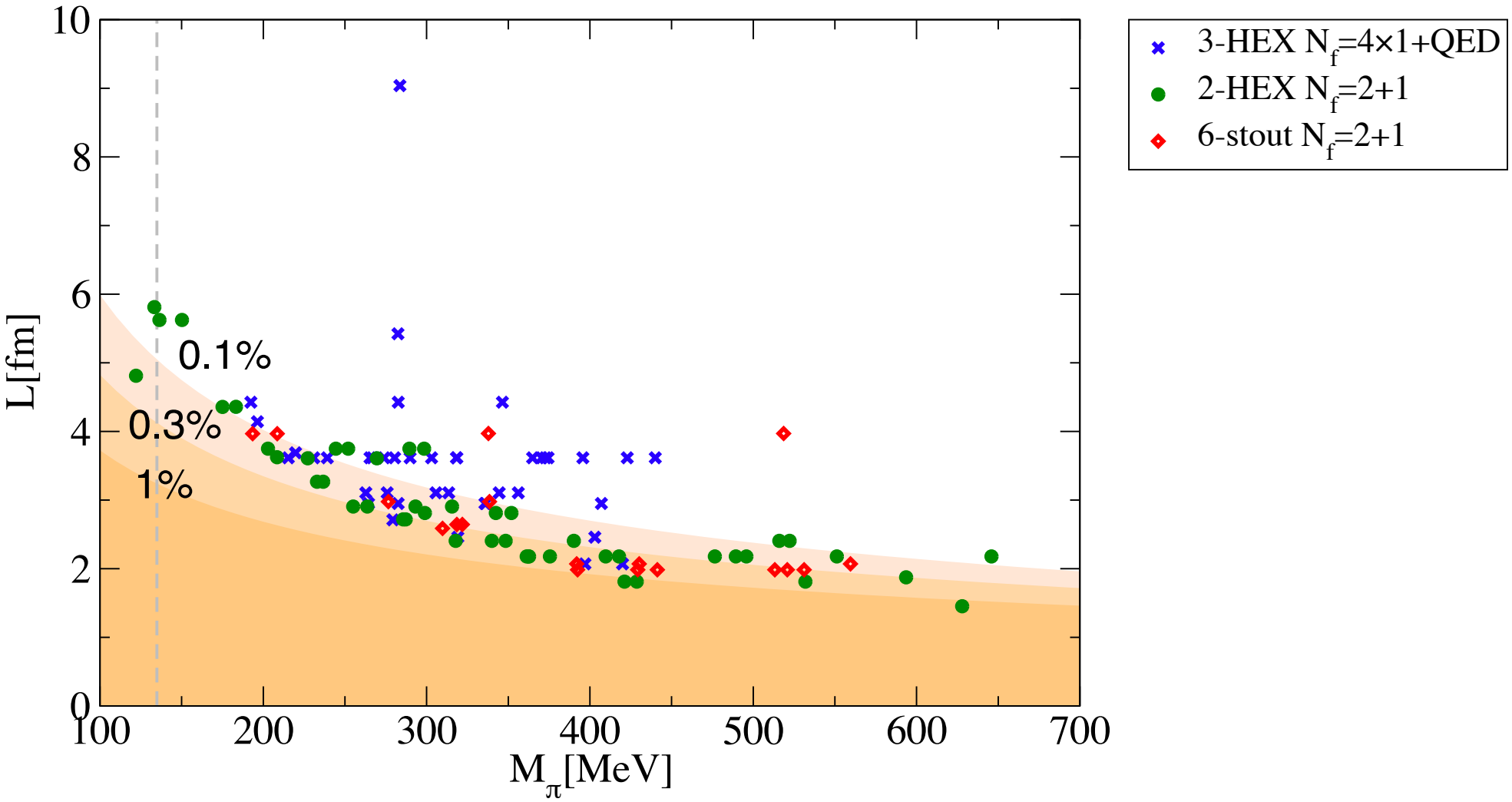
Method:

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

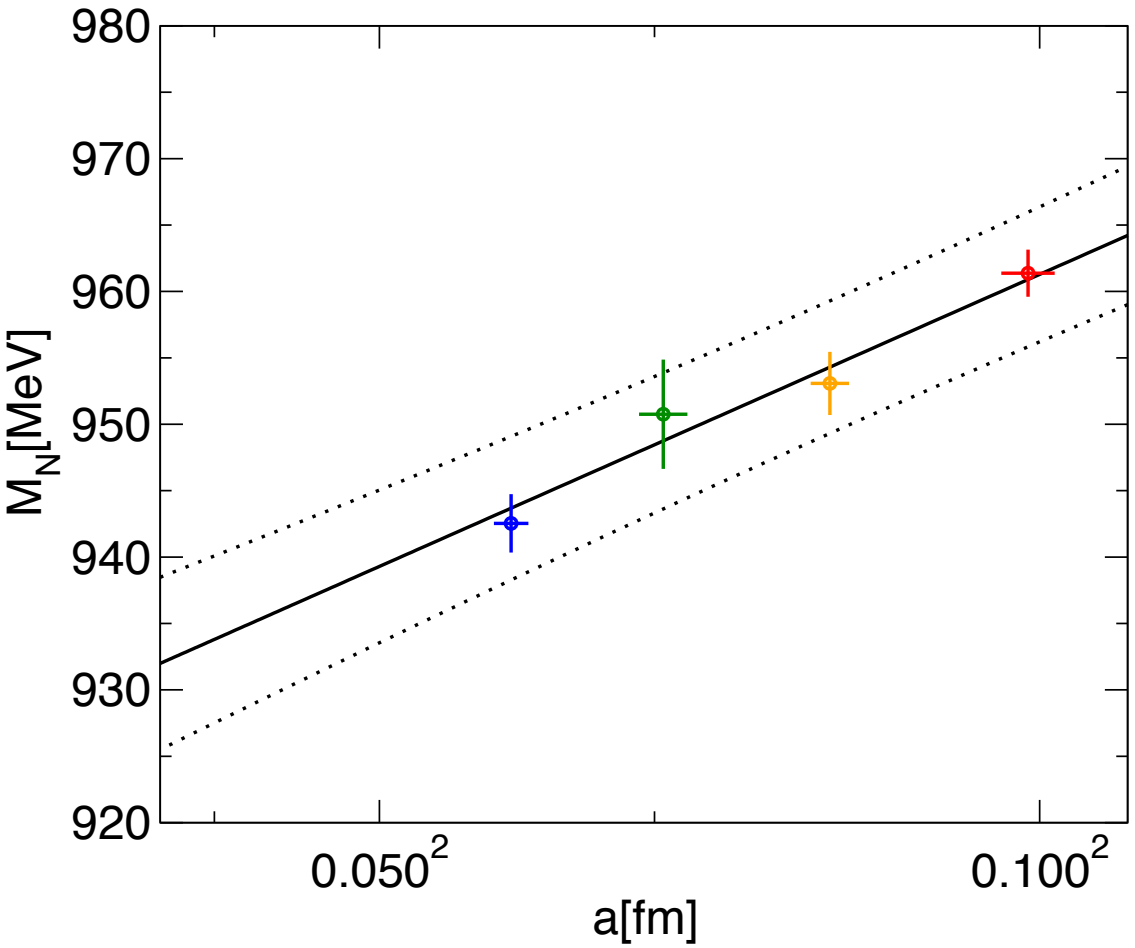




Landscape L vs. M_π



Continuum limit



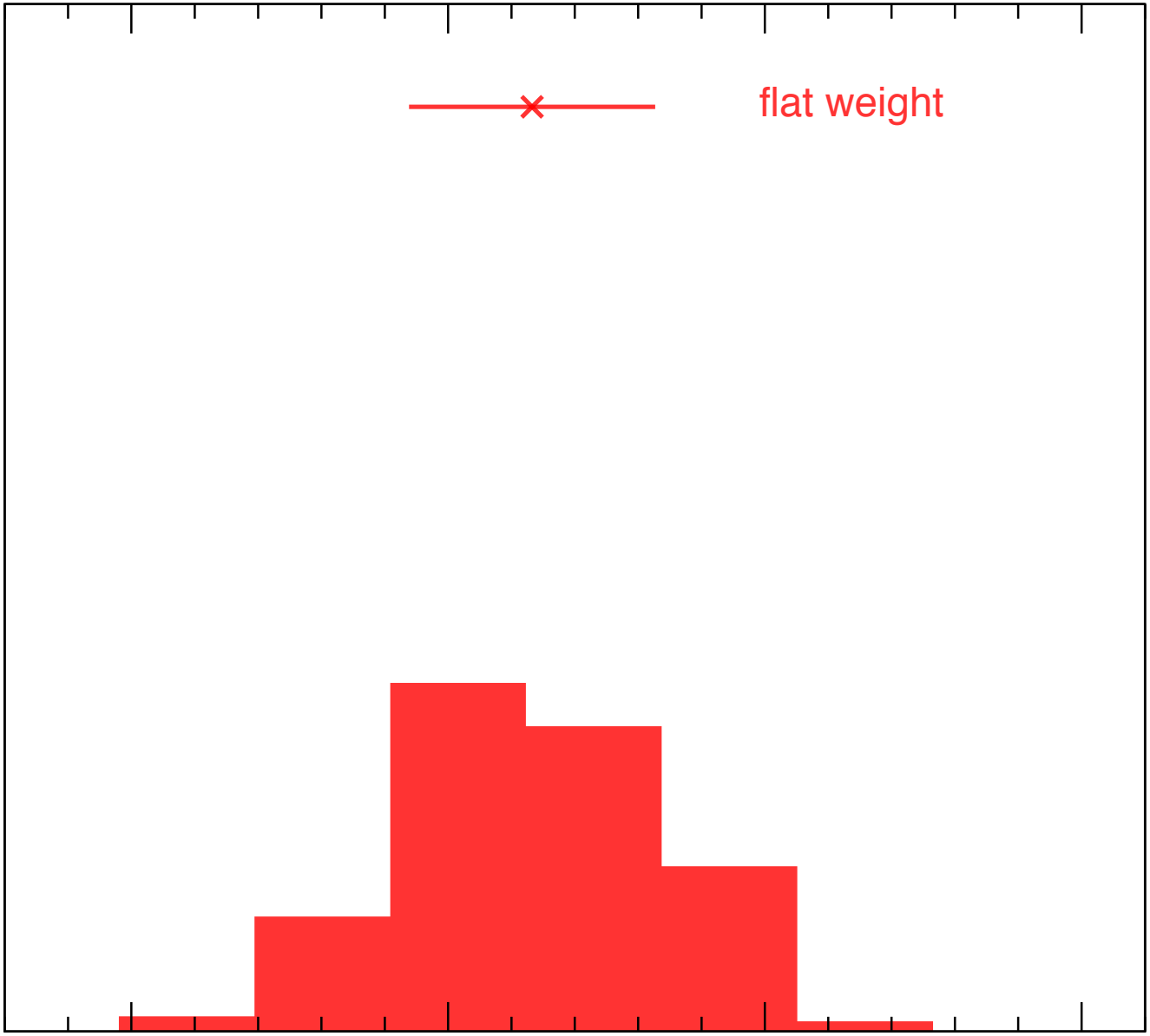
- Formally $O(\alpha a)$
- Subleading $O(a^2)$ can be dominant
- Use both, difference into systematics

Systematic error treatment

One conservative strategy for systematics:

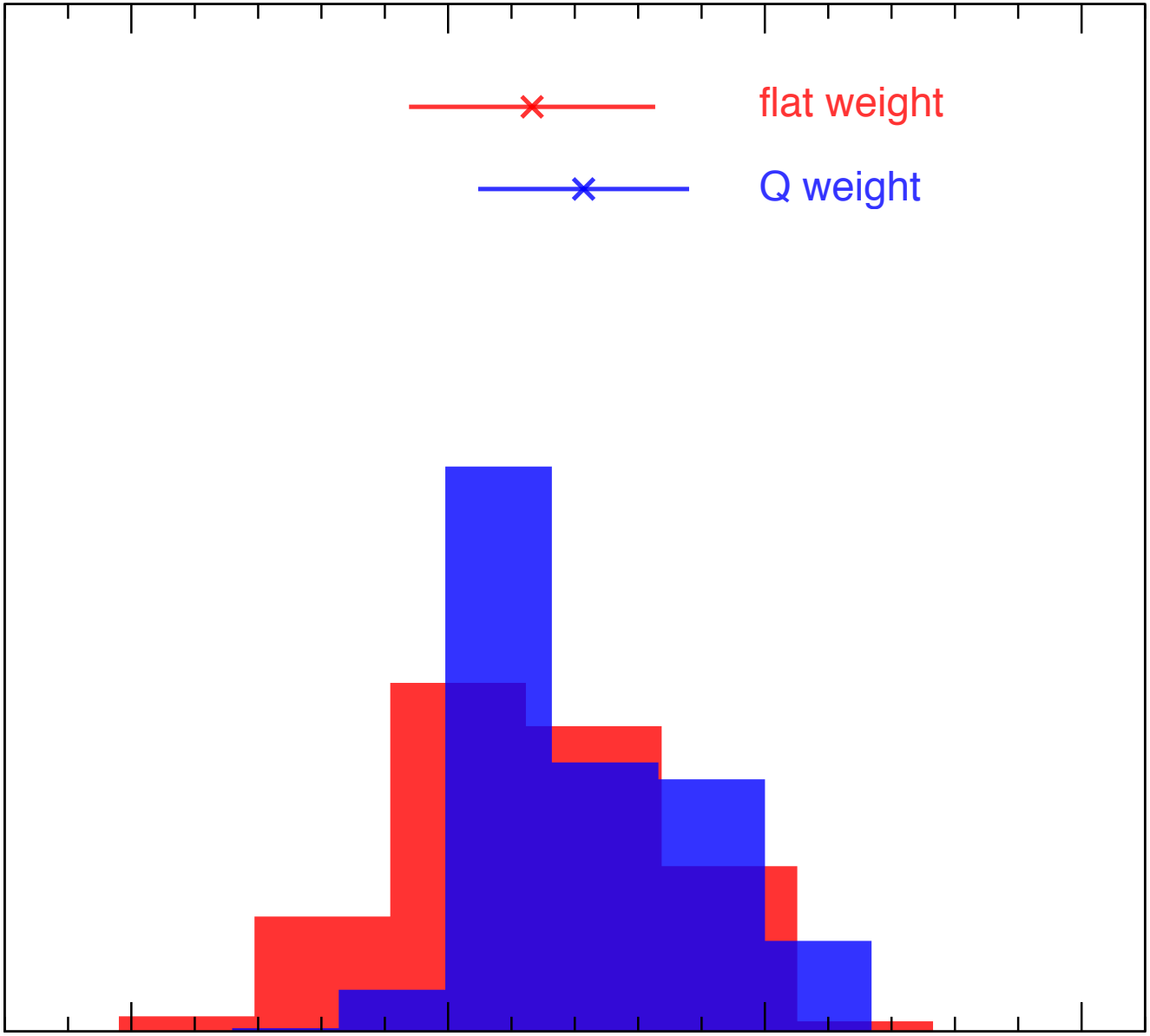
- Identify all higher order effects you have to neglect
- For each of them:
  - Repeat the entire analysis treating this one effect differently
  - Add the spread of results to systematics
- Important:
  - Do not do suboptimal analyses
  - Do not double-count analyses
- Error sources considered:
  - 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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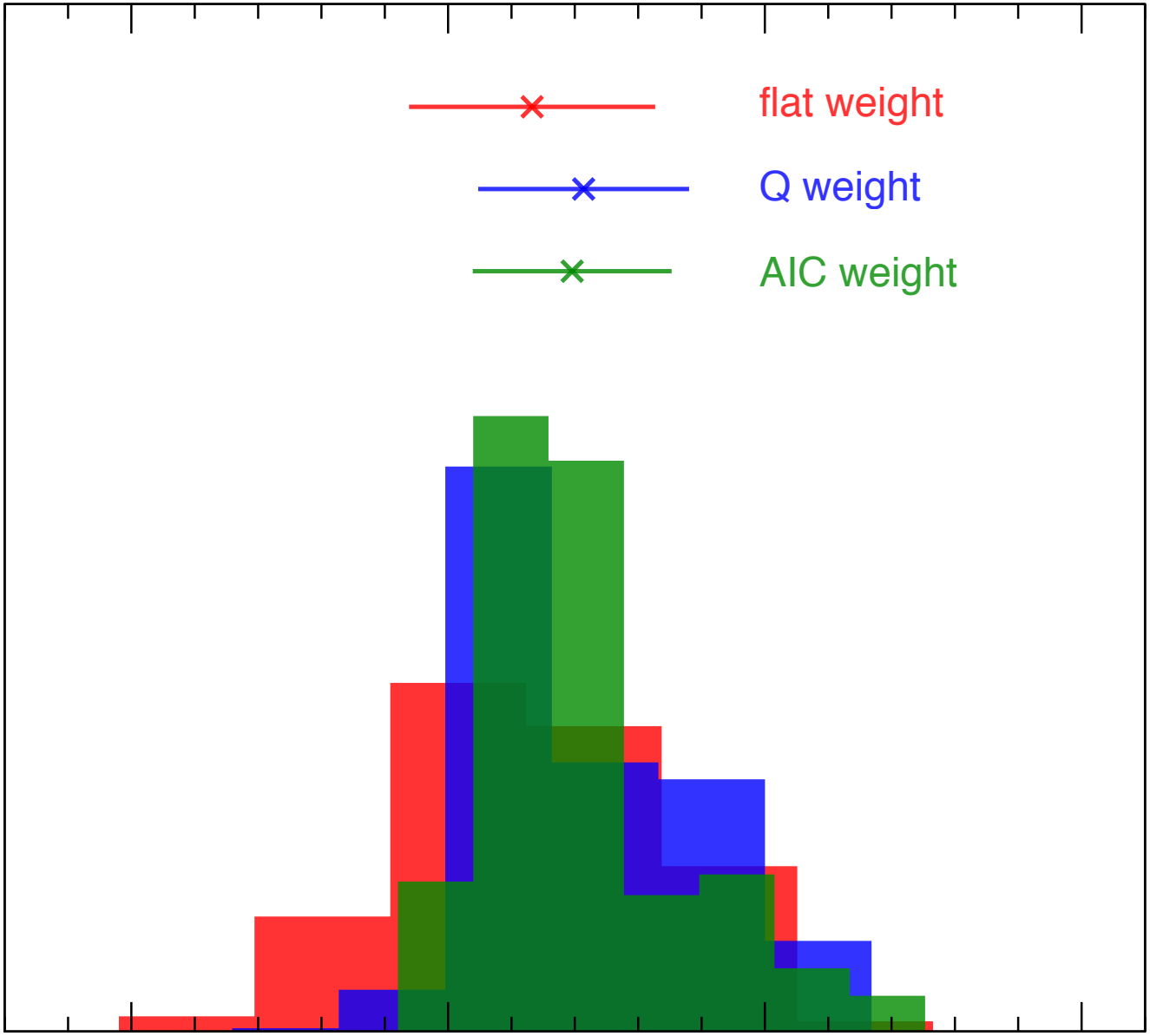

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From the effective Hamiltonean

$$H = H_{\text{iso}} + \frac{\delta m}{2} \int d^3x (\bar{d}d - \bar{u}u)$$

we obtain (with $\delta m = m_d - m_u$)

$$\Delta_{QCD} M_N = \frac{\delta m}{2M_p} \langle p|\bar{u}u - \bar{d}d|p\rangle$$

which, together with

$$f^p_{u/d} = \left(\frac{1}{2} \mp \frac{\delta m}{4m_{ud}}\right) f^p_u d + \left(\frac{1}{4} \mp \frac{m_{ud}}{2\delta m}\right) \frac{\delta m}{2M_p^2} \langle p|\bar{d}d - \bar{u}u|p\rangle$$

gives ($r = m_u/m_d$)

$$f_u^{p/n} = \left(\frac{r}{1+r}\right) f^N_{ud} \pm \frac{1}{2}\left(\frac{r}{1-r}\right) \frac{\Delta_{QCD} M_N}{M_N} + O(\delta m^2, m_{ud}\delta m)$$

$$f_d^{p/n} = \left(\frac{1}{1+r}\right) f^N_{ud} \mp \frac{1}{2}\left(\frac{1}{1-r}\right) \frac{\Delta_{QCD} M_N}{M_N} + O(\delta m^2, m_{ud}\delta m)$$

Results (BMWc, 2015)

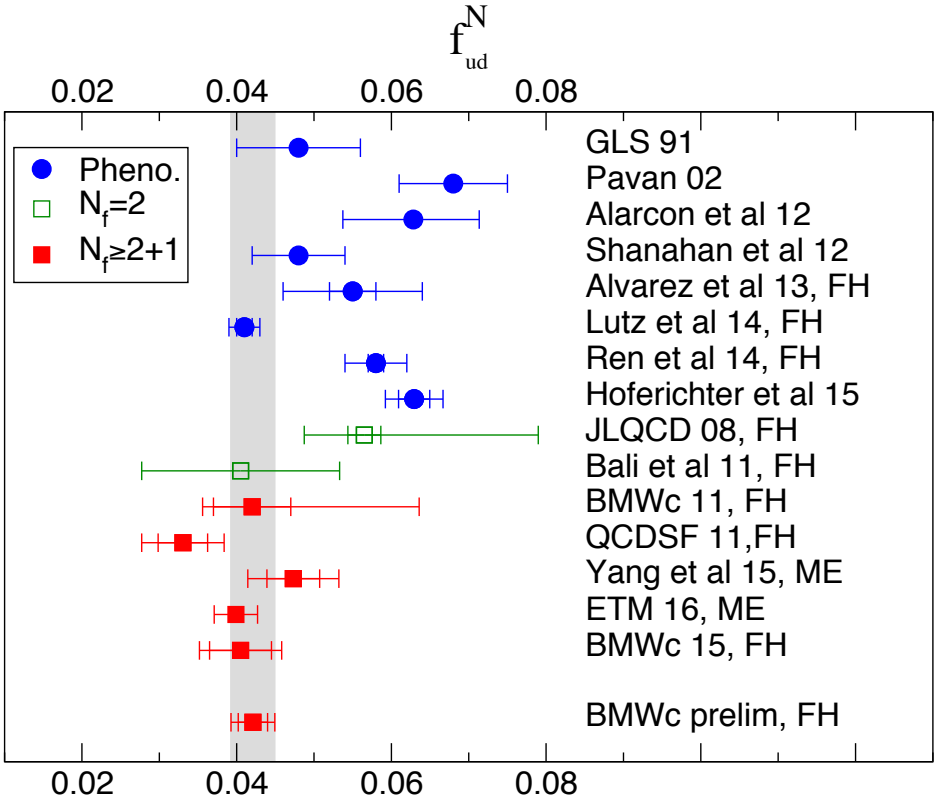
Direct results:

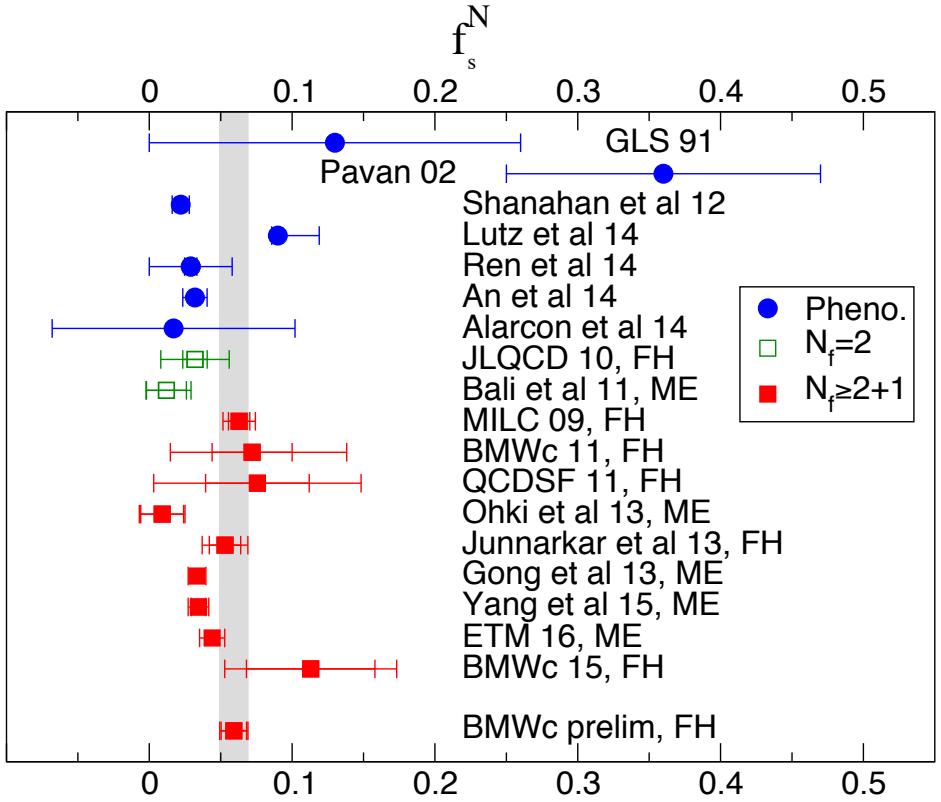
$$f_{ud}^N = 0.0405(40)(35) \qquad \sigma_{ud}^N = 38(3)(3)\text{MeV}$$
$$f_s^N = 0.113(45)(40) \qquad \sigma_s^N = 105(41)(37)\text{MeV}$$

With $\Delta_{QCD} M_N = 2.52(17)(24)\text{MeV}$ from (BMWc 2014)

$$f_u^p = 0.0139(13)(12) \qquad f_d^p = 0.0253(28)(24)$$
$$f_u^n = 0.0116(13)(11) \qquad f_d^n = 0.0302(28)(25)$$

PRELIMINARY result on new dataset





$$f_{ud}^N = 0.0421(19)(20) \qquad f_s^N = 0.0592(89)(43)$$

PRELIMINARY result on new dataset

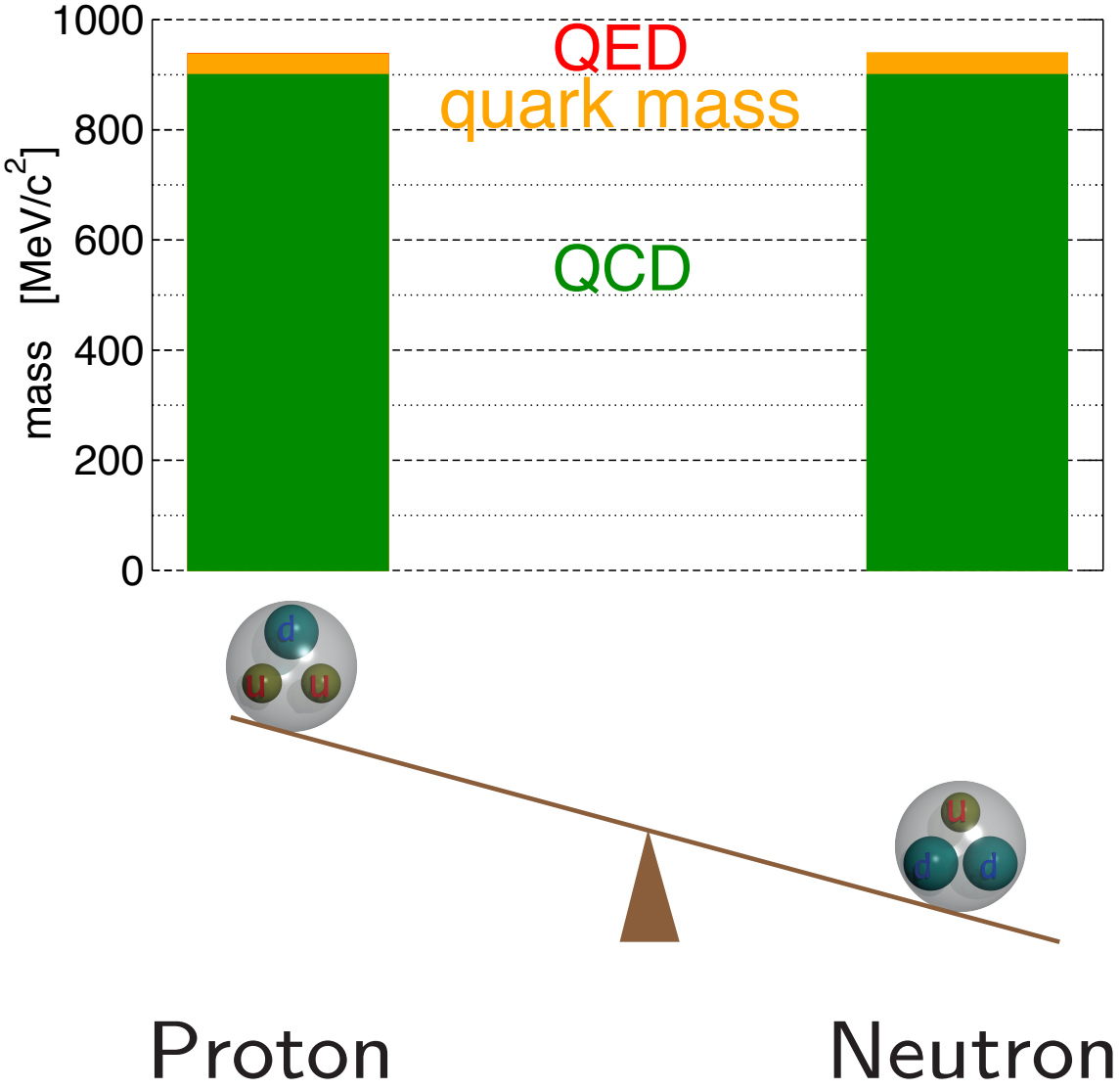
$$M_N = 937(12)(4)\text{MeV}$$

$$M_N|_{m_{ud}=0, m_s \text{ const.}} = 896(13)(5)\text{MeV} \quad \sigma_{ud}^N = 39.5(1.4)(1.8)\text{MeV}$$

$$M_N|_{m_s=0, m_{ud} \text{ const.}} = 881(13)(4)\text{MeV} \quad \sigma_s^N = 55.5(5.5)(4.1)\text{MeV}$$

BACKUP

IS THE FINE STRUCTURE RELEVANT?



- 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

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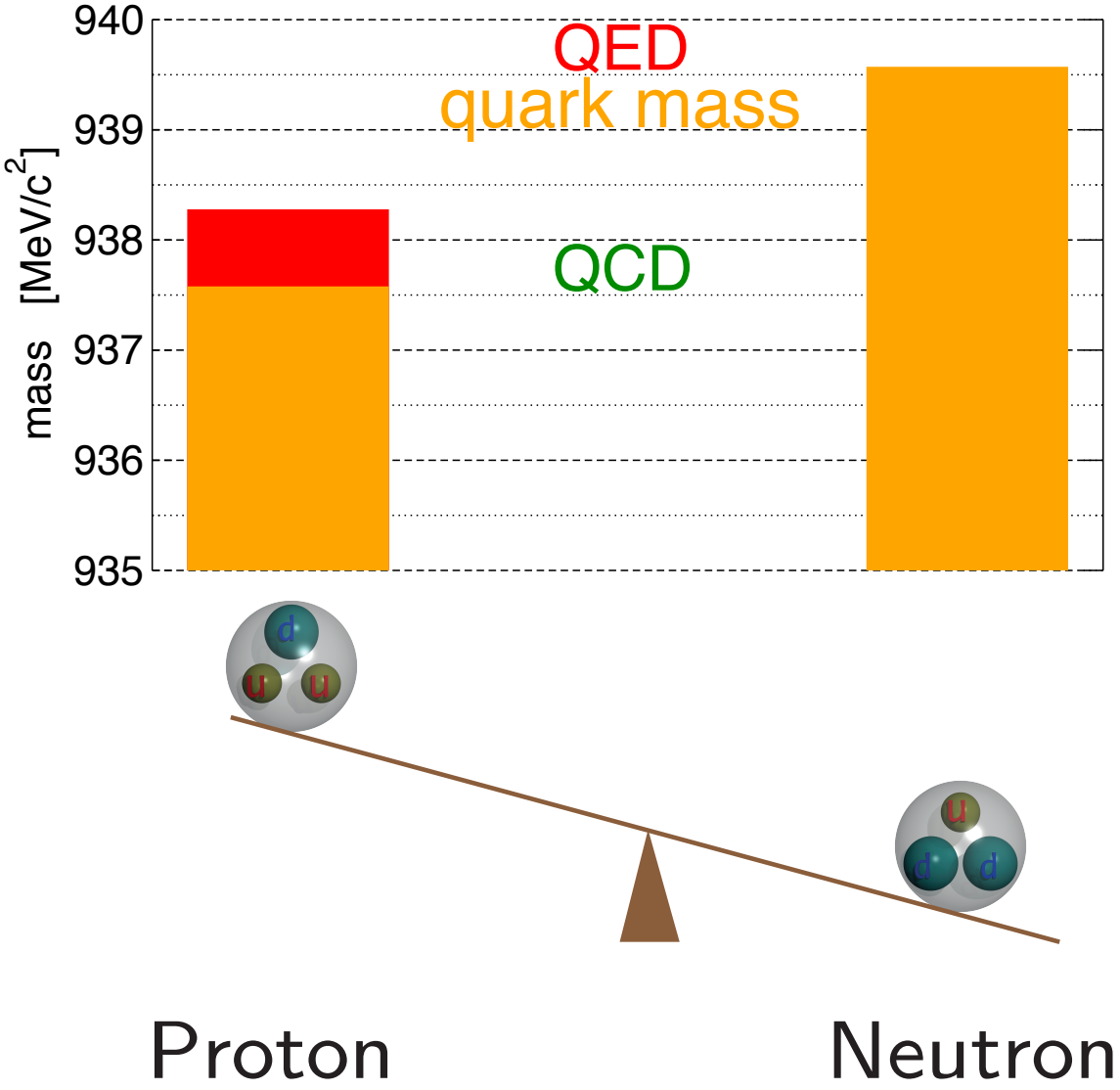

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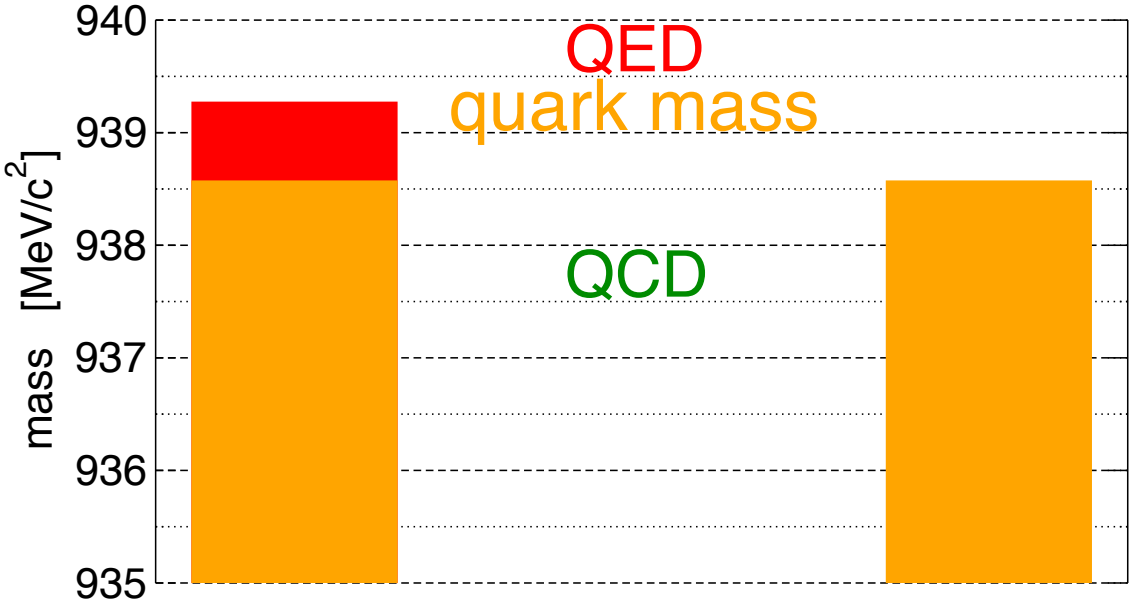

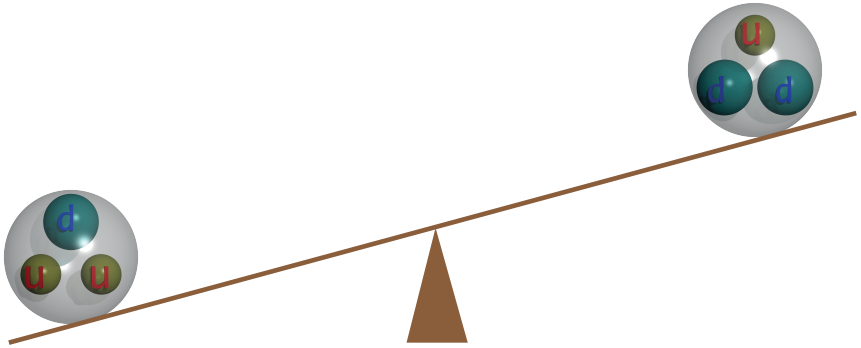

Proton Neutron

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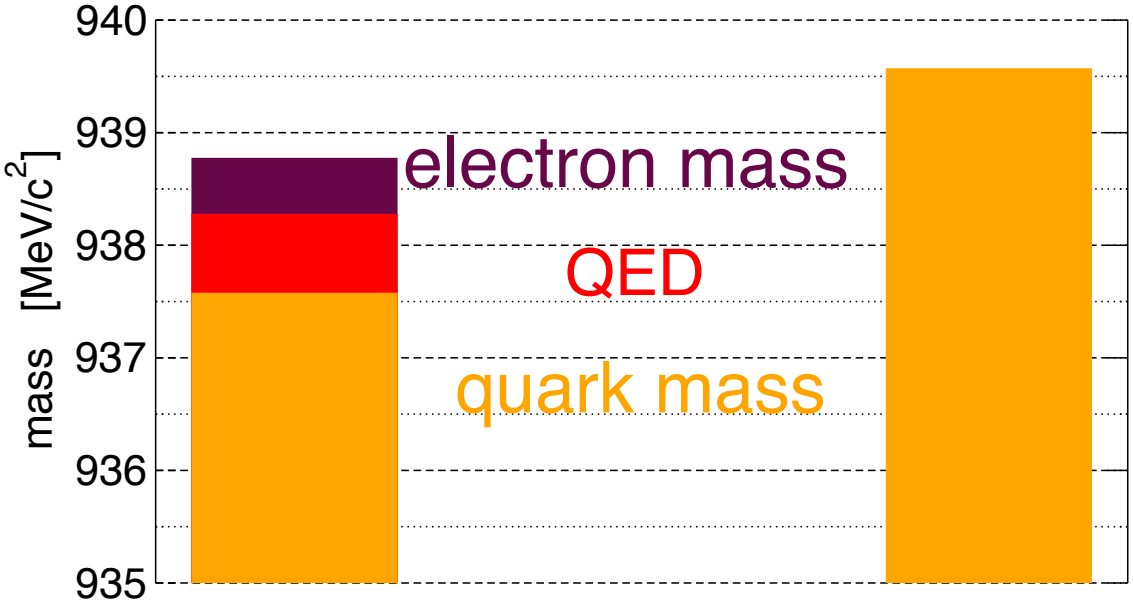

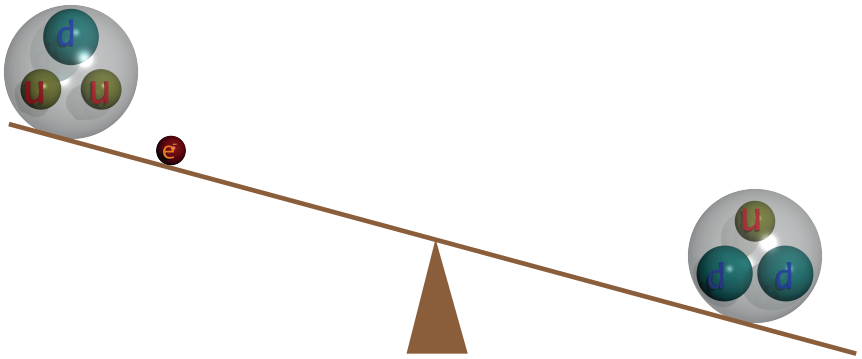

Proton Neutron

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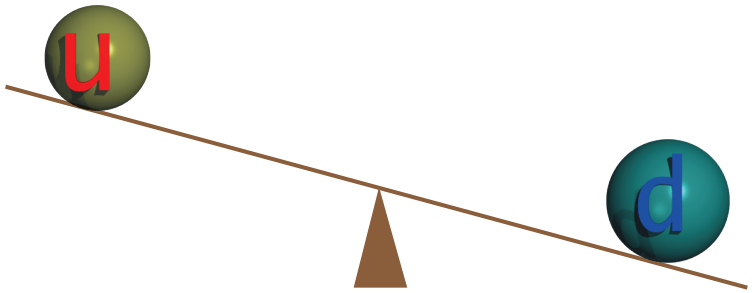
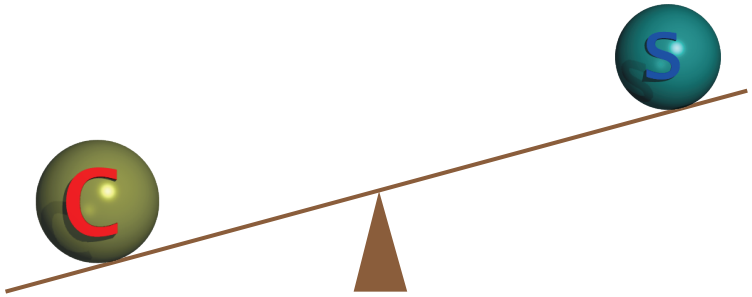
ANTHROPIC PUZZLE? THE LIGHT UP QUARK

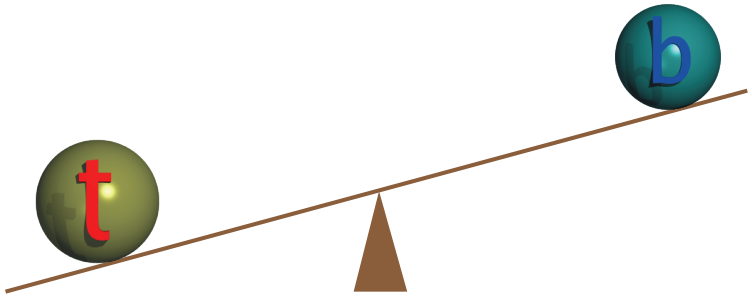


1st generation: $m_u < m_d$

Why?

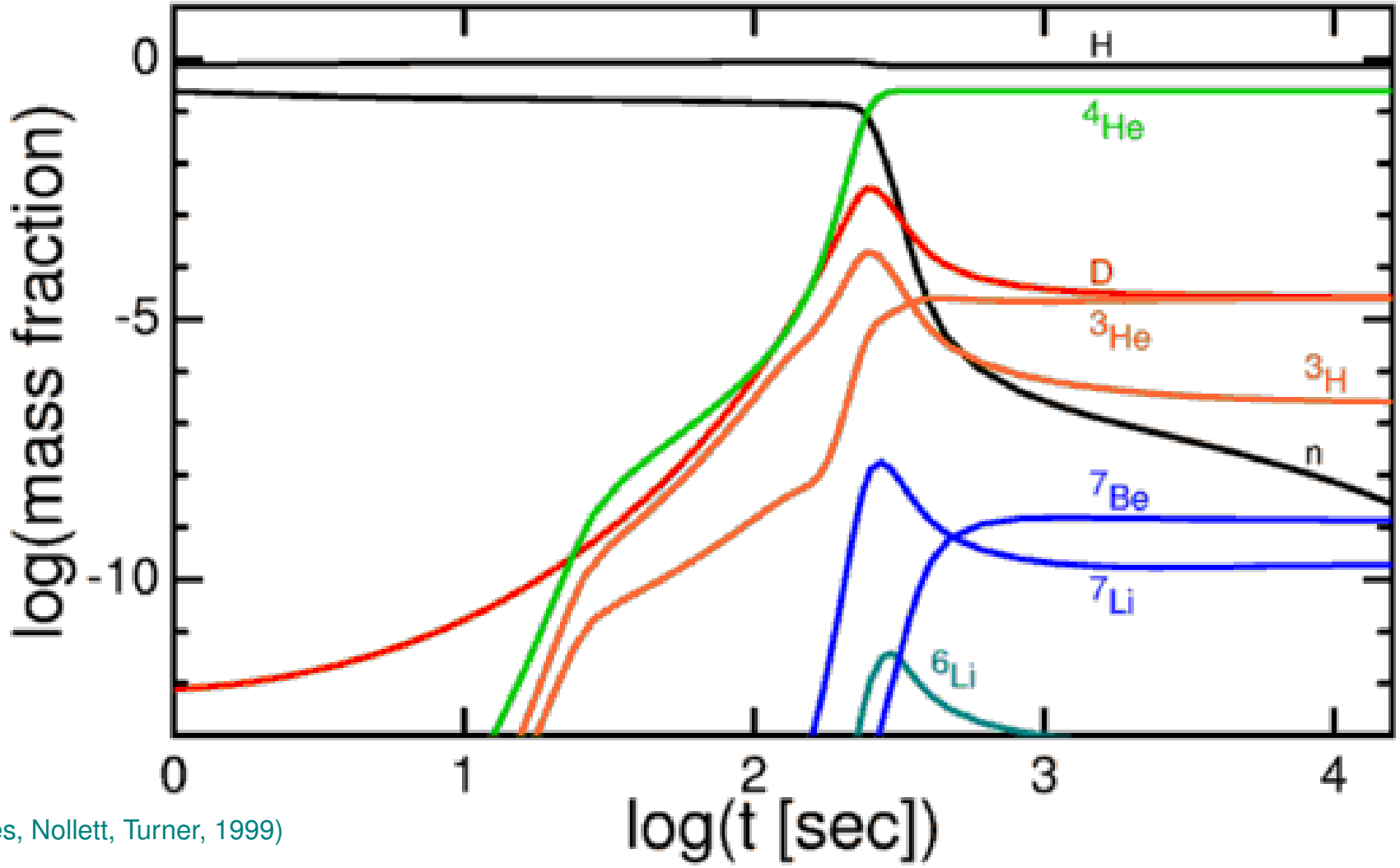


2nd generation: $m_c > m_s$



3rd generation: $m_t > m_b$

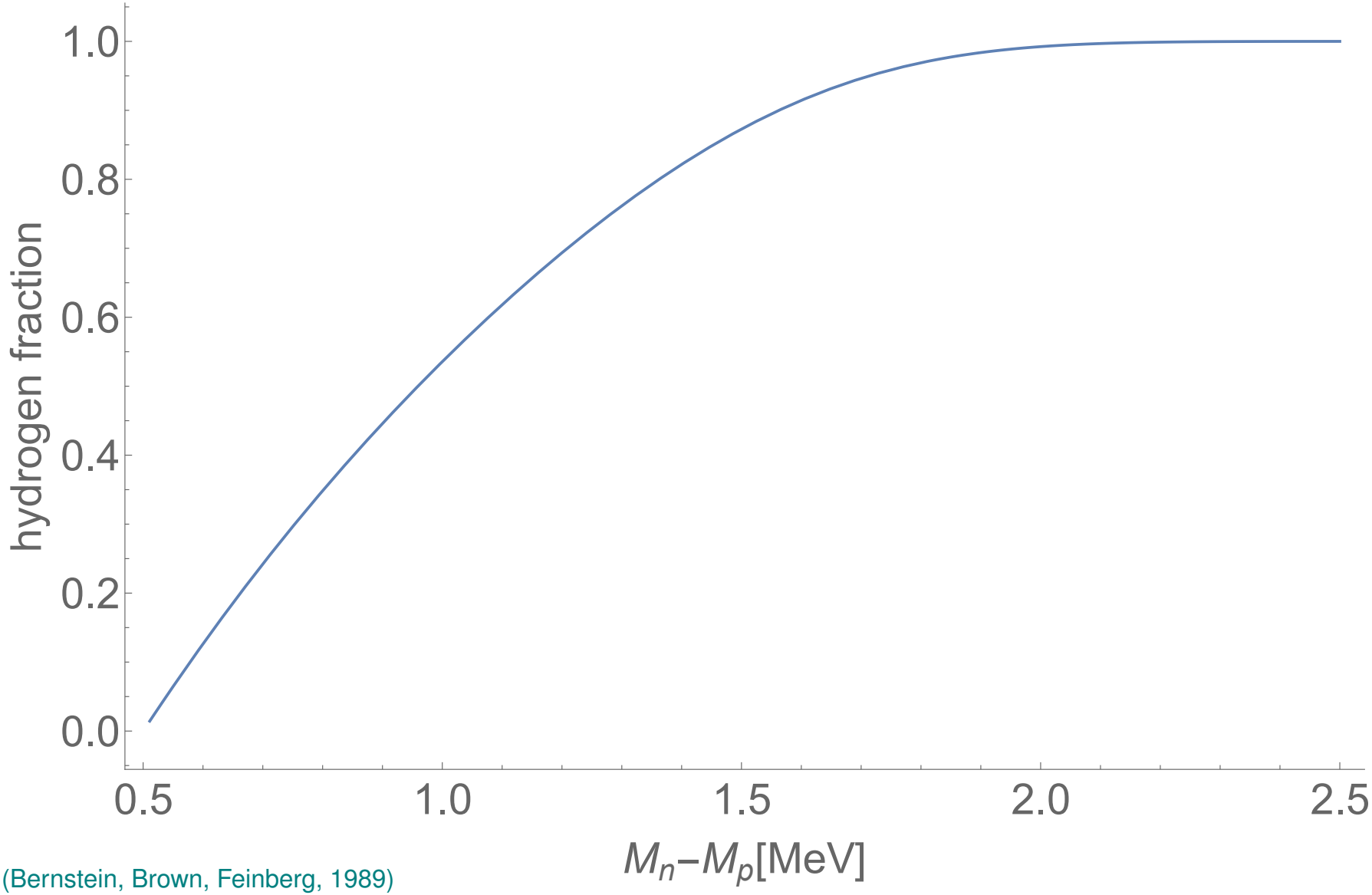
Big bang nucleosynthesis



(Burles, Nollett, Turner, 1999)

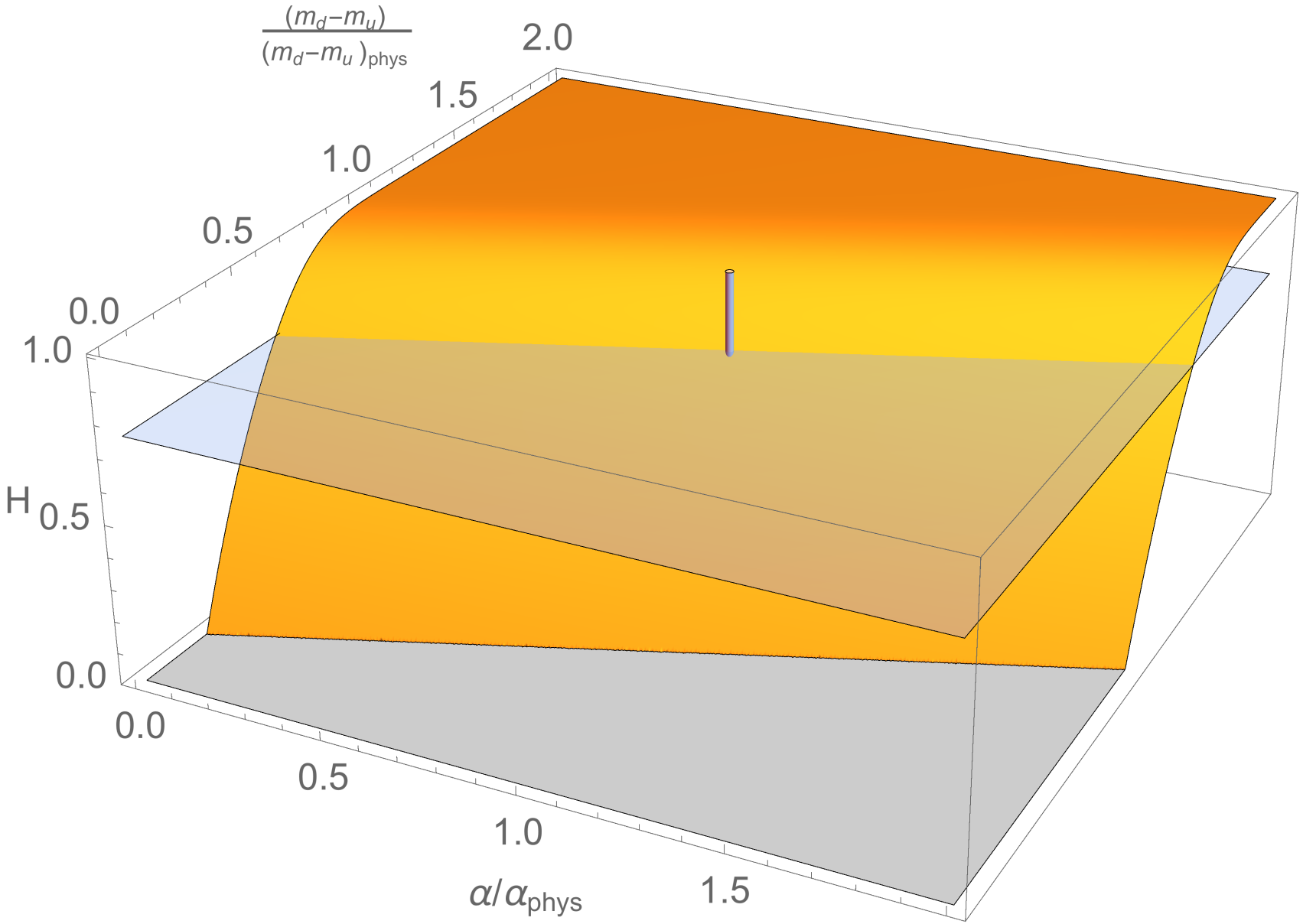
$M_n - M_p$ determines deuterium bottleneck

Hydrogen abundance



(Bernstein, Brown, Feinberg, 1989)

Resulting initial hydrogen abundance



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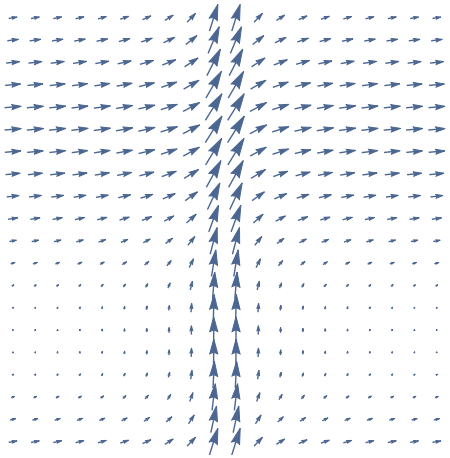
$$\lim_{\xi(t) \to 0} \int dt \frac{1}{\xi(t)} \left(\int d^3 x A_\mu(x) \right)^2$$

  - Transfer matrix exists



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

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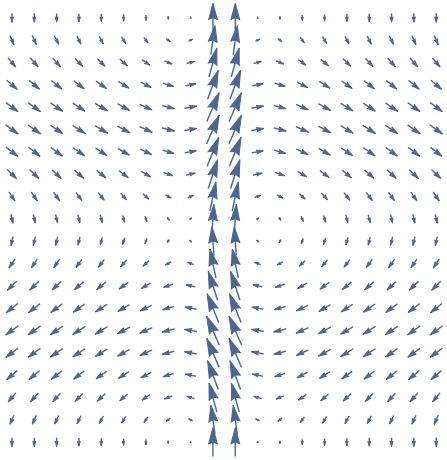

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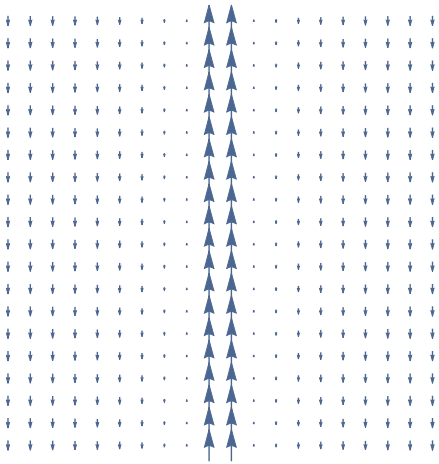

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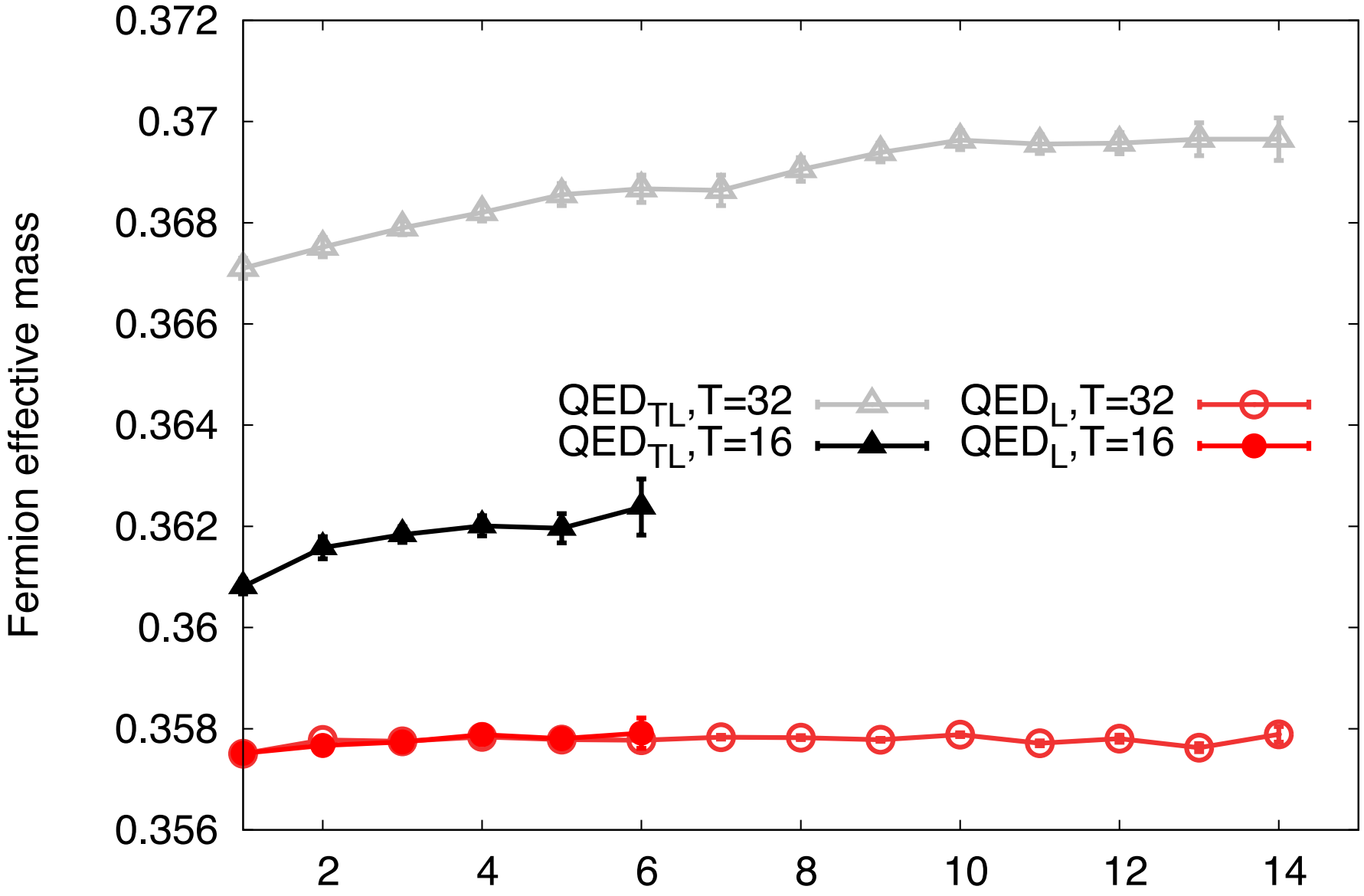
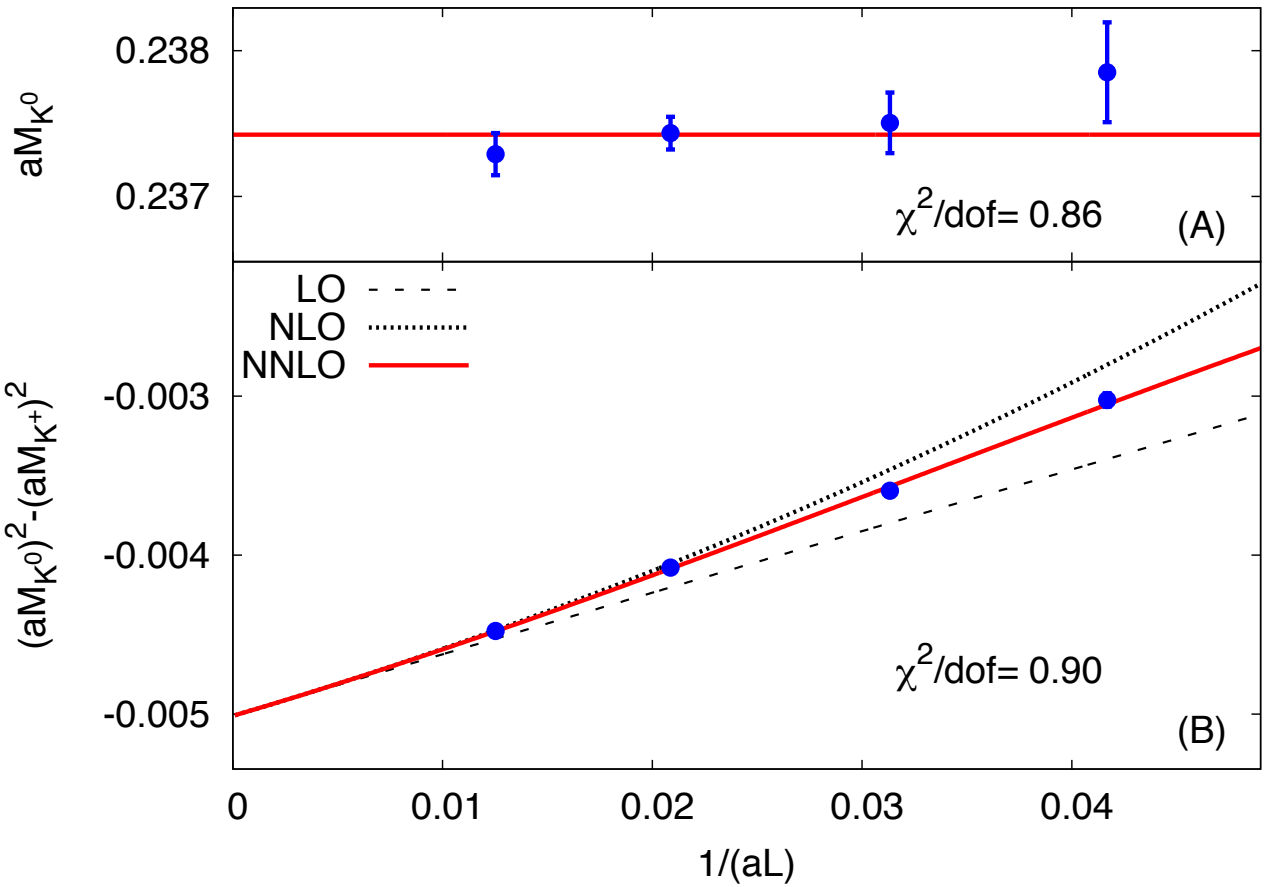
Quenched QED FV effects



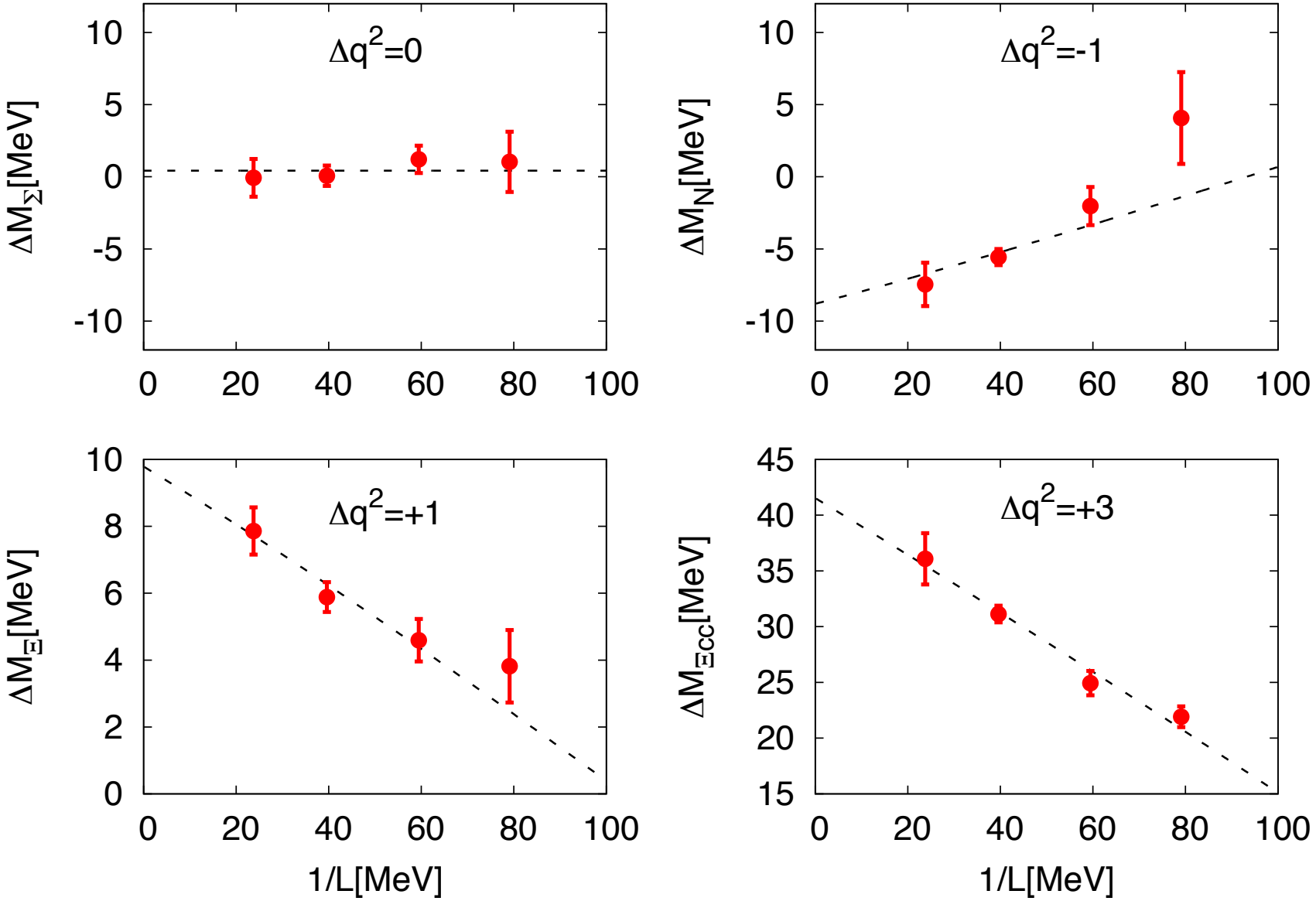
Universal FV effects



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

(BMWc, 2014)

Baryon FV in QCD+QED



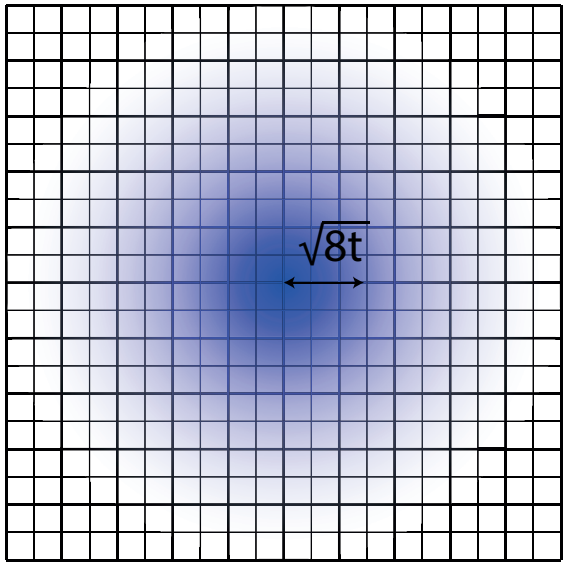
Identifying the physical point

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

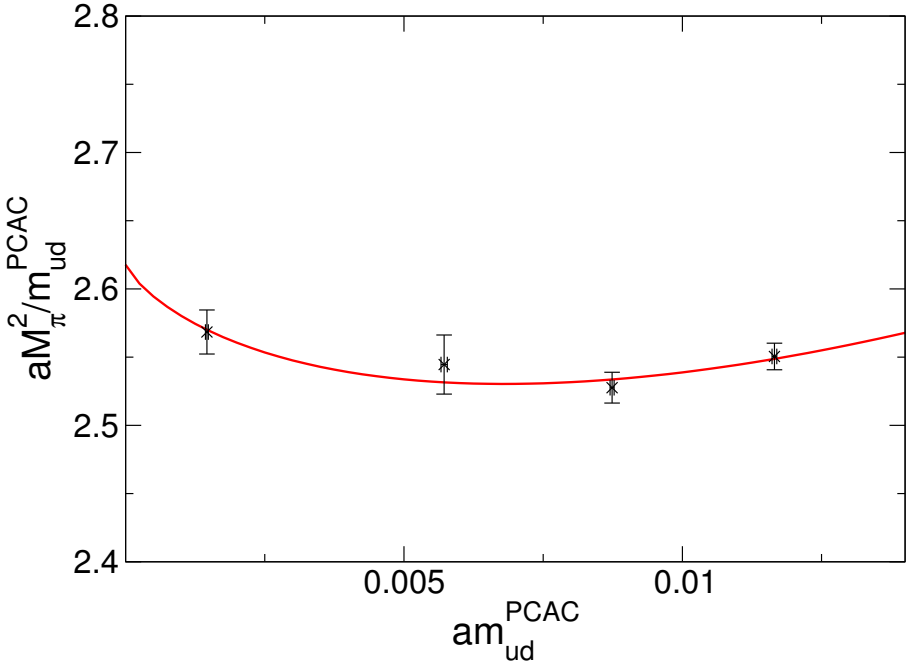
$$\langle F_{\mu\nu} F_{\mu\nu} \rangle = \frac{6}{V_4} \sum_k e^{-2|\hat{k}|^2 t}$$

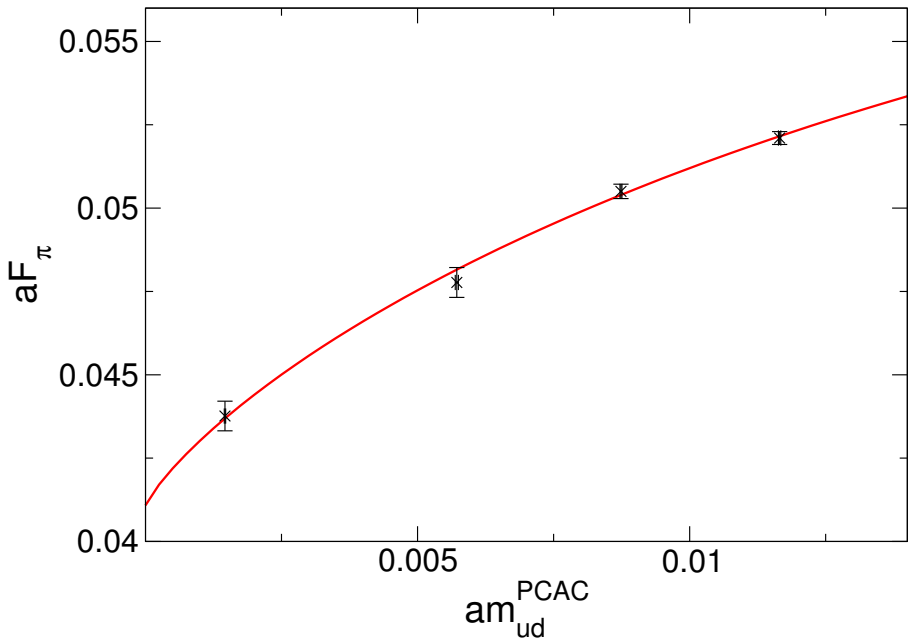
Slightly more complicated for clover plaquette



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

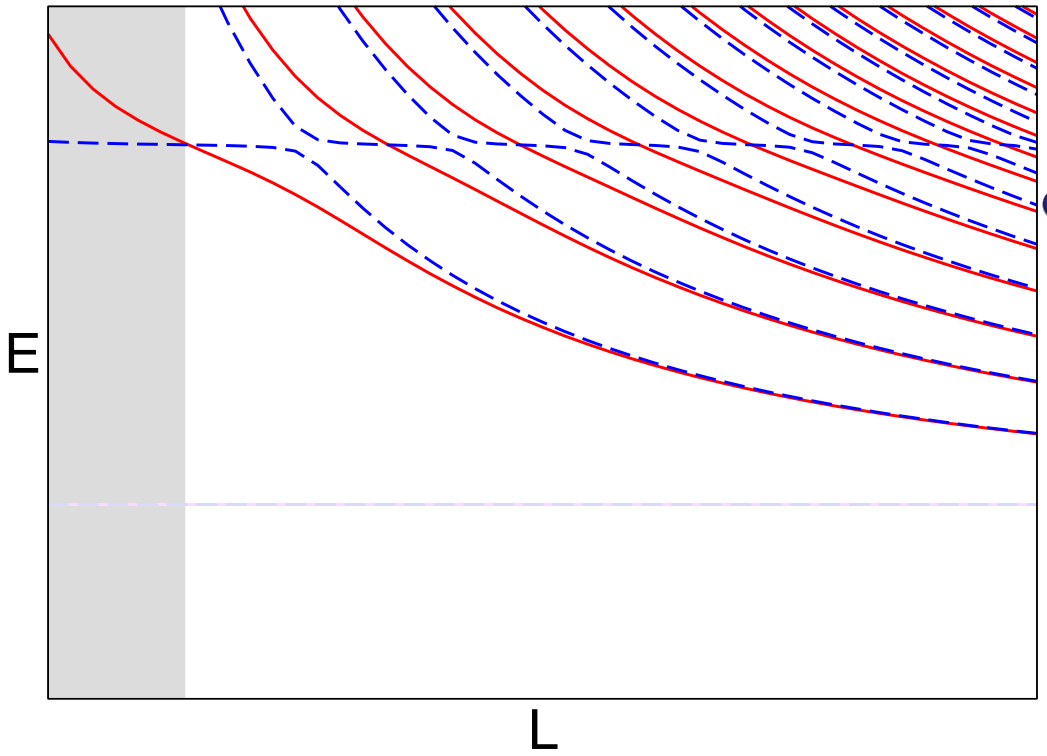
Finite volume effects in resonances

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

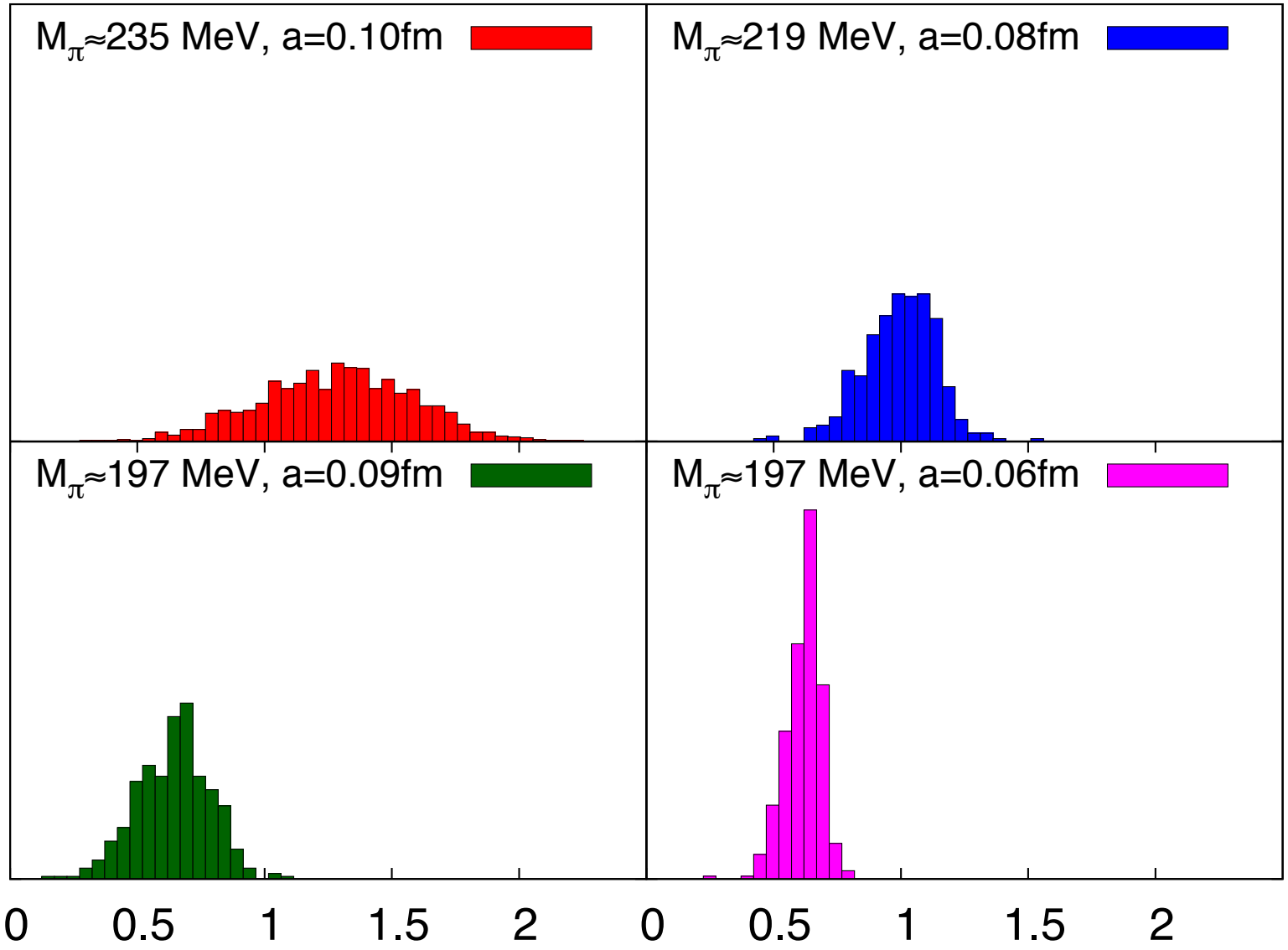


- Treatment as scattering problem

  (Lüscher, 1985-1991)

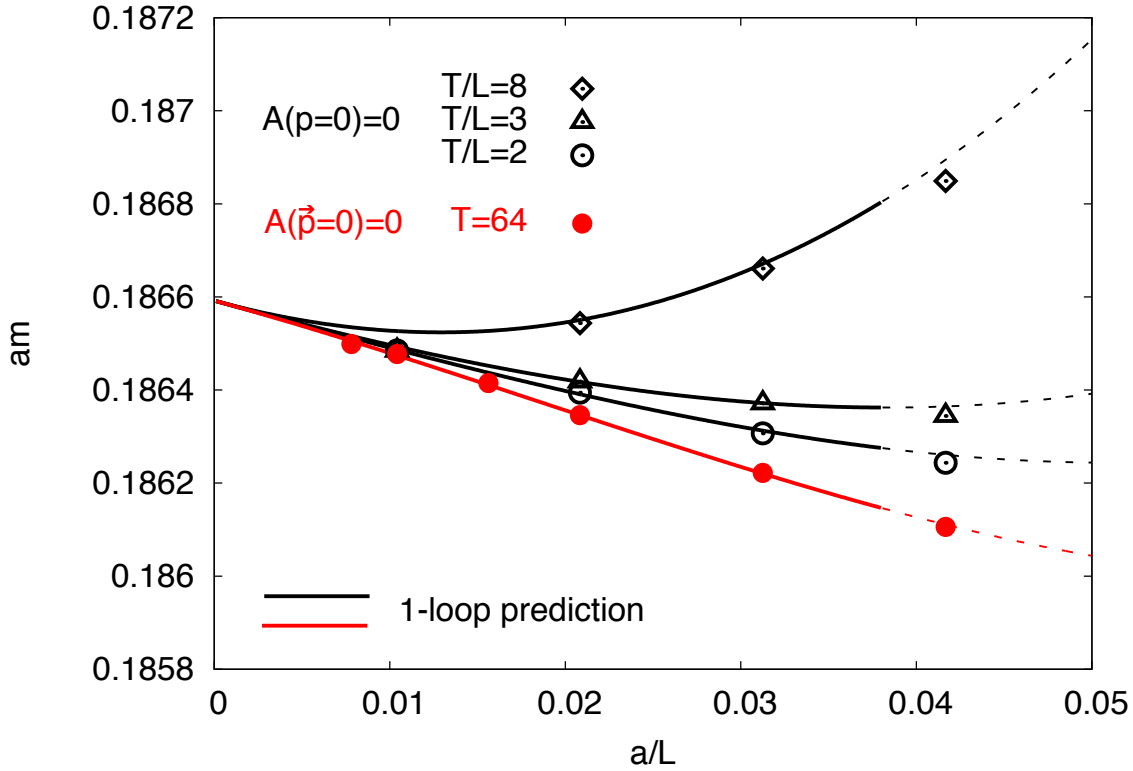
  - Parameters: mass and coupling (width)
  - Alternative approaches suggested

No exceptional configurations



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



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

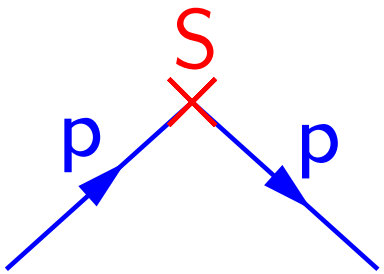
(BMWc, 2014)

Renormalization

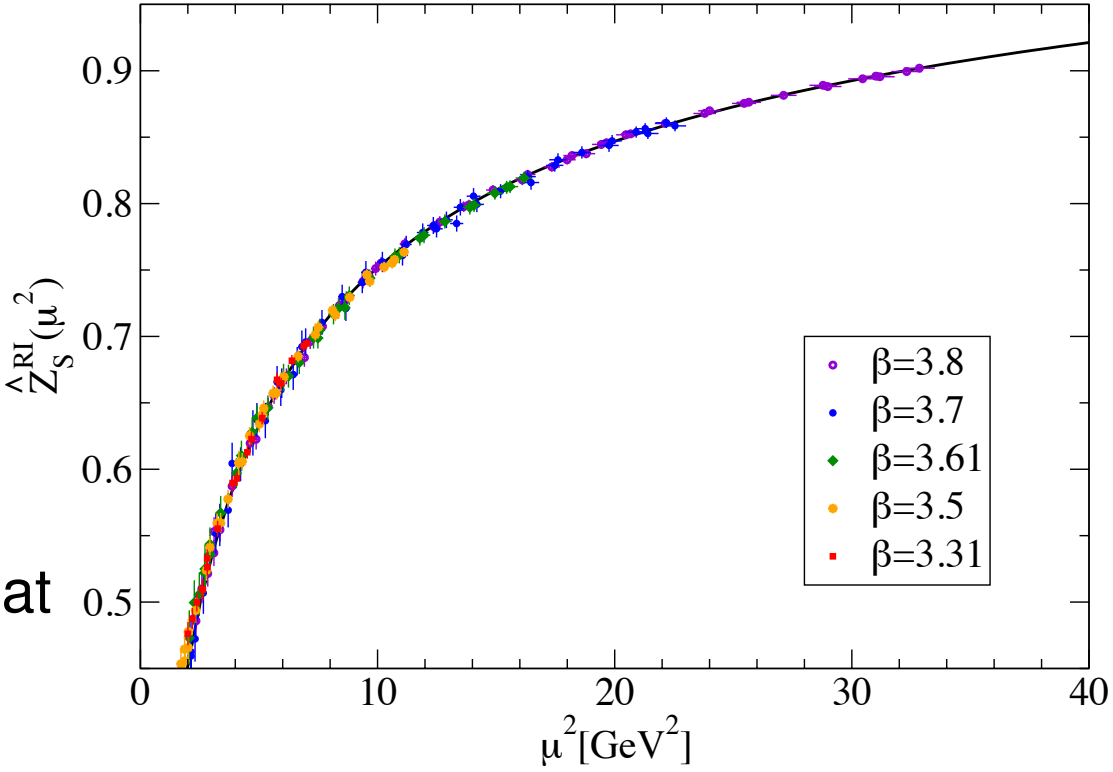
- Quark masses logarithmically divergent ($a \to 0$) ➛ renormalization
- Usual scheme $\overline{\text{MS}}$: perturbatively defined

☞ RI-MOM scheme

- Matrix elements of off-shell quarks in fixed gauge



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



Quark mass definitions

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

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

Better use

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

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

and reconstruct

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

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

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

✓ Only Z_S multiplicative renormalization (no pion poles)

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

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	publication status	chiral extrapolation	continuum extrapolation	finite volume	renormalization	running	m_{ud}	m_s
PACS-CS 10	P	★	■	■	★	a	2.78(27)	86.7(2.3)
MILC 10A	C	●	★	★	●	–	3.19(4)(5)(16)	–
HPQCD 10	A	●	★	★	★	–	3.39(6)*	92.2(1.3)
BMW 10AB	P	★	★	★	★	b	3.469(47)(48)	95.5(1.1)(1.5)
RBC/UKQCD	P	●	●	★	★	c	3.59(13)(14)(8)	96.2(1.6)(0.2)(2.1)
Blum et al. 10	P	●	■	●	★	–	3.44(12)(22)	97.6(2.9)(5.5)

(FLAG, 2011)

Masses of the u and d quarks

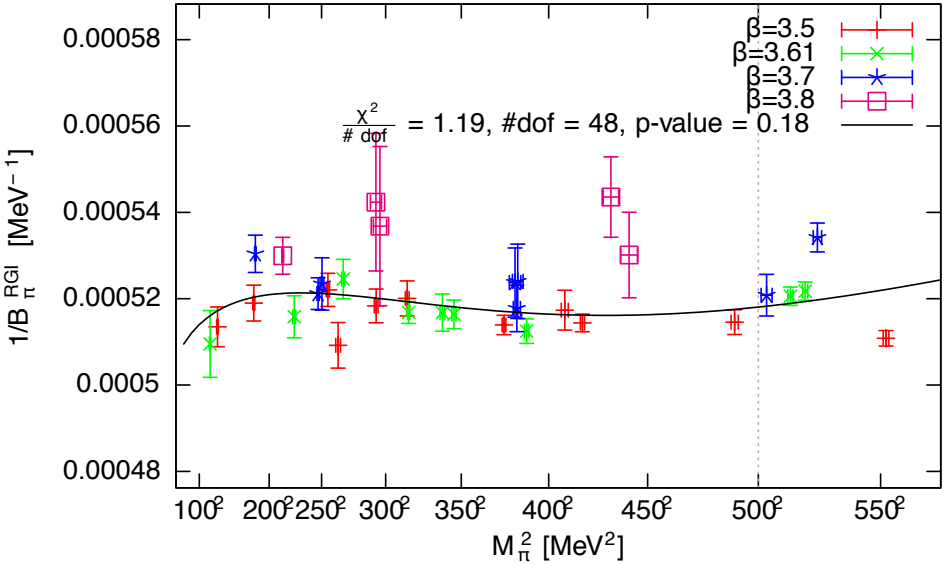
Goal:

- Directly compute m_u and m_d

Method:

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

Computing $m_u - m_d$:

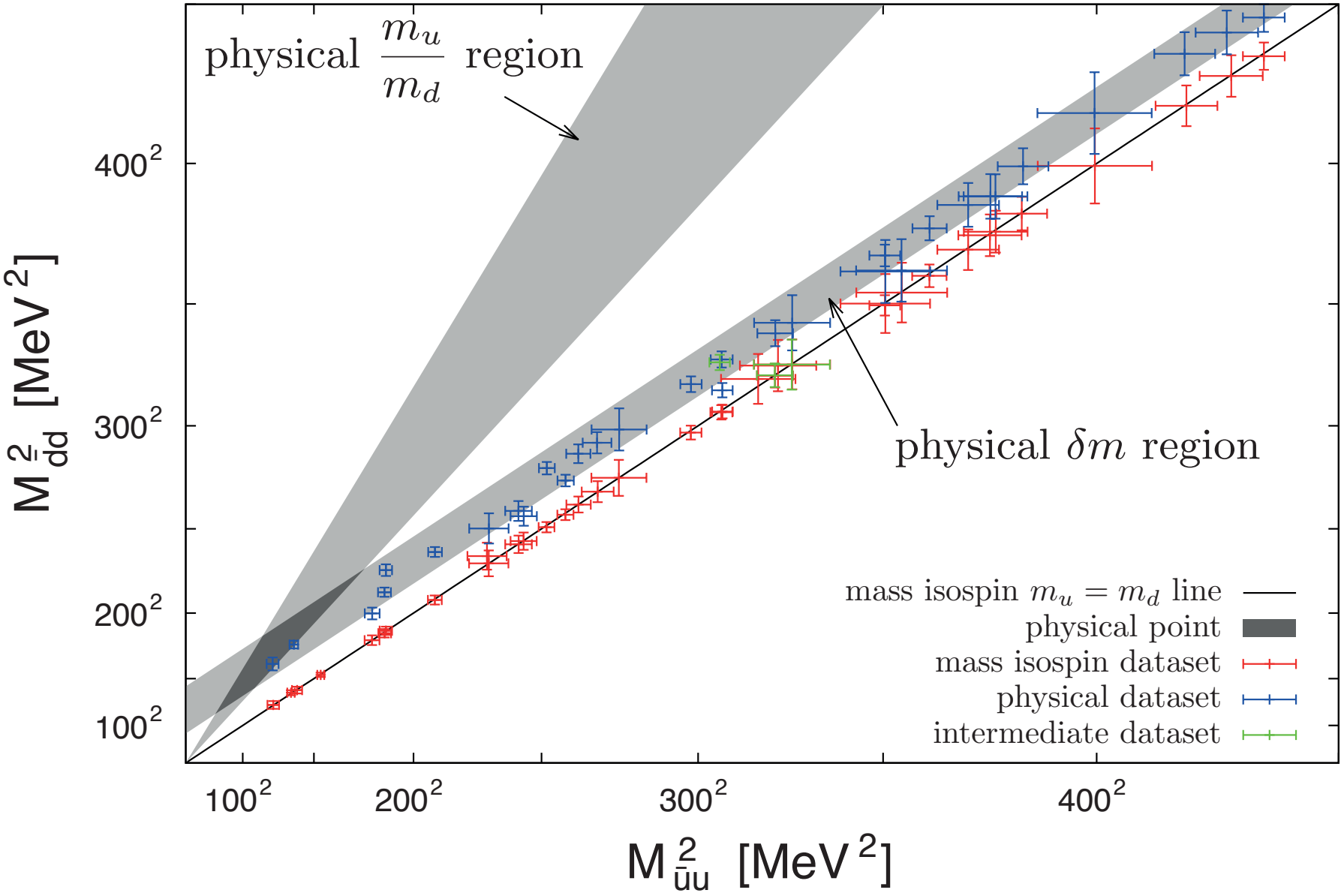


- Parameterize $\delta m = m_u - m_d$ via $\Delta M^2 = M_{uu}^2 - M_{dd}^2$

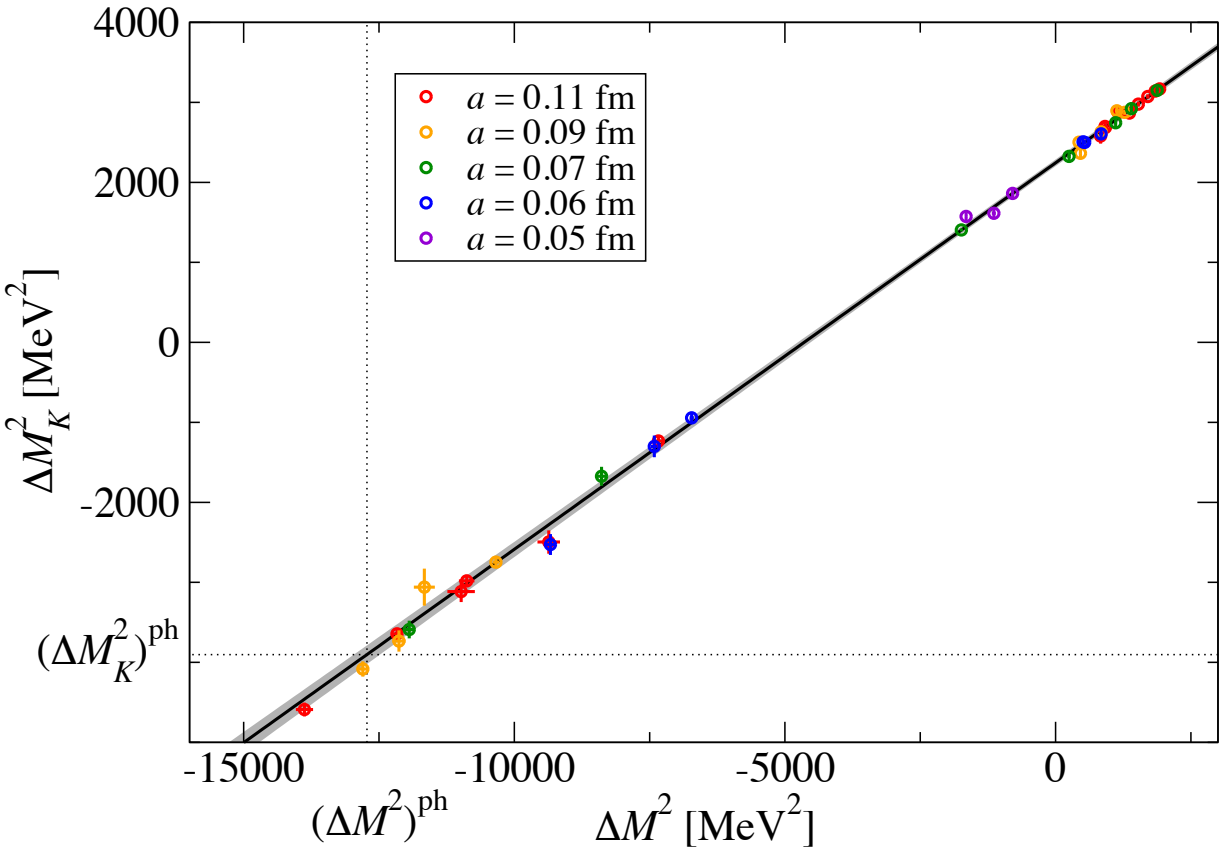
$$\Delta M^2 = 2B_2\delta m + O(m_{ud}\alpha, m_{ud}\delta m, \alpha^2, \alpha\delta m, \delta m^2)$$

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

Extracting physical ΔM^2

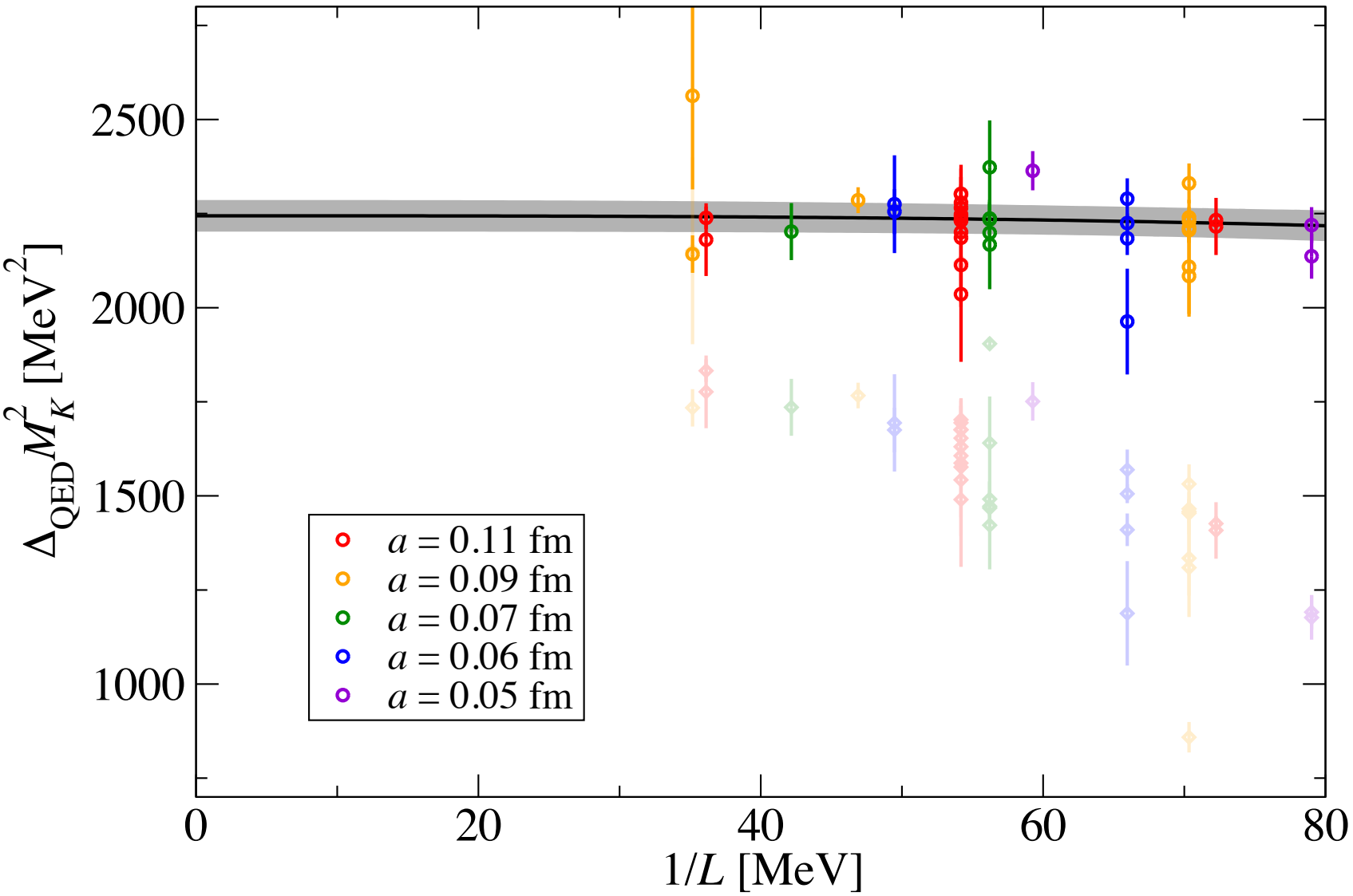


$$\Delta M_K^2 = \Delta M^2 C_X + \alpha D_X$$

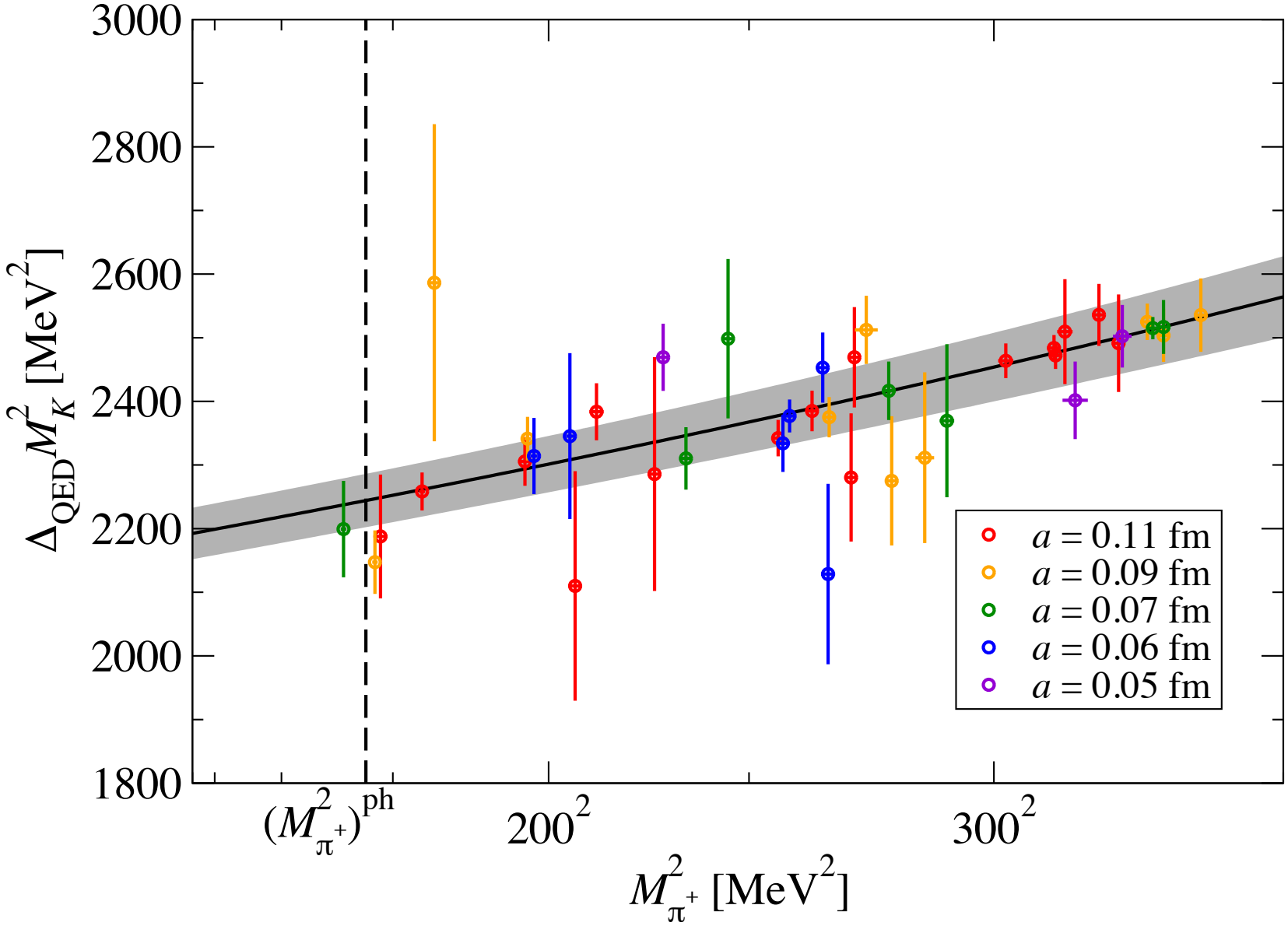
$$C_X = c_X^0 + c_X^1 \hat{M}_\pi^2 + c_X^2 \hat{M}_K^2 + c_X^3 f(a)$$

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

Finite volume



Chiral interpolation



Results

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

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