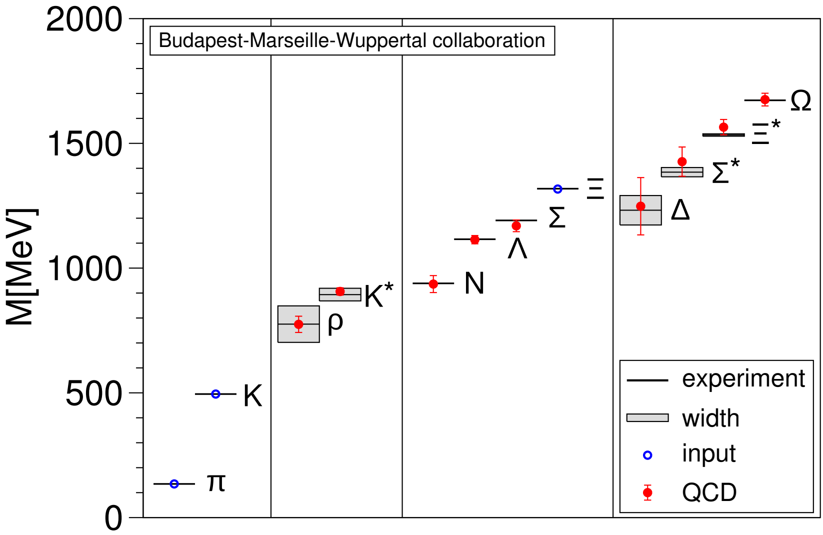
Ab initio computation of the proton-neutron mass difference

Sz. Borsanyi, S. Dürr, Z. Fodor, Christian Hoelbling, S. Katz, S. Krieg, L. Lellouch, T. Lippert, A. Portelli, K. Szabo, B. Toth

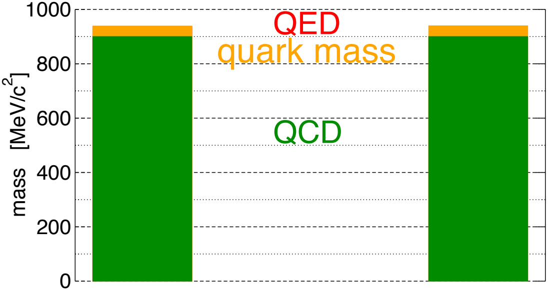
Budapest-Marseille-Wuppertal collaboration

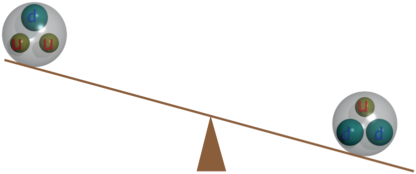
Science 347 (2015) 1452
[arXiv:1406.4088]

THE LIGHT HADRON SPECTRUM



IS THE FINE STRUCTURE RELEVANT?



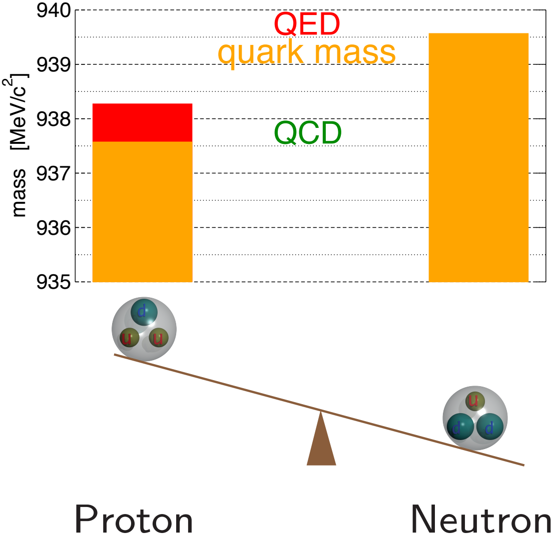


Proton Neutron

- 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

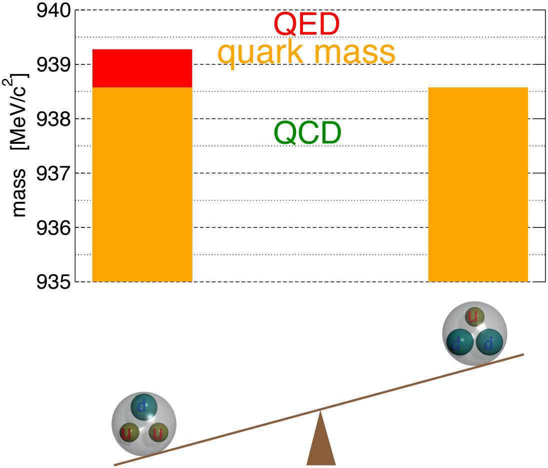
IS THE FINE STRUCTURE RELEVANT?



- 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

IS THE FINE STRUCTURE RELEVANT?

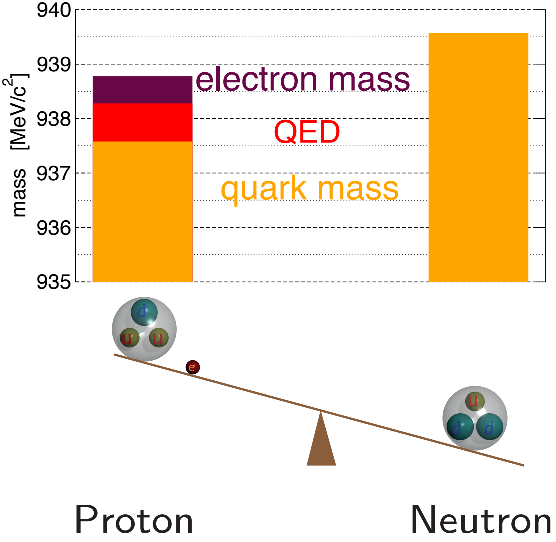


Proton Neutron

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

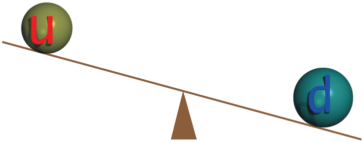
- $m_u < m_d : M_p < M_n$
- $m_u = m_d : M_p > M_n$ Proton decays
- $M_p + M_{e^-} \gtrsim M_n$ No hydrogen

IS THE FINE STRUCTURE RELEVANT?



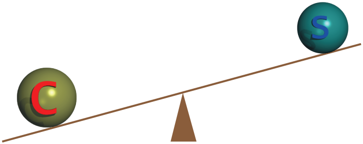
- Proton, neutron: 3 quarks
- Proton: uud
- Neutron: udd
- $m_u < m_d : M_p < M_n$
- $m_u = m_d : M_p > M_n$ Proton decays
- $M_p + M_{e^-} \gtrsim M_n$ No hydrogen

ANTHROPIC PUZZLE? THE LIGHT UP QUARK

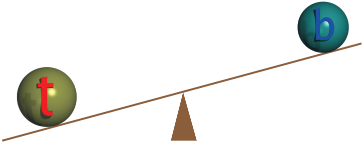


1st generation: $m_u < m_d$

Why?

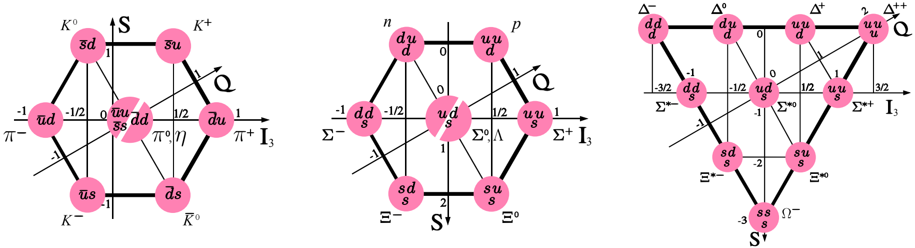


2nd generation: $m_c > m_s$



3rd generation: $m_t > m_b$

SOURCES OF ISOSPIN SPLITTING



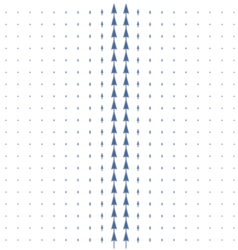
- Two sources of isospin breaking:
  - QCD: $\sim \frac{m_d - m_u}{\Lambda_{QCD}} \sim 1\%$
  - QED: $\sim \alpha(Q_u - Q_d)^2 \sim 1\%$
- On the lattice:
  - Include nondegenerate light quarks $m_u \neq m_d$
  - Include QED

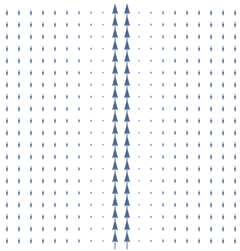
CHALLENGES OF QED SIMULATIONS

- 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)





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

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

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

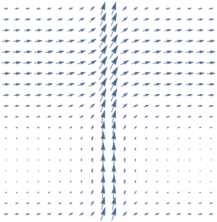
- Removing momentum modes with measure 0 as $V \to \infty$ allowed
- Remove $k = 0$ from momentum sum (QED_{TL})
  - Realised by a constraint term in the action

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

  - 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

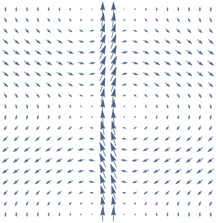
- Removing momentum modes with measure 0 as $V \to \infty$ allowed
- Remove $k = 0$ from momentum sum (QED_{TL})
  - Realised by a constraint term in the action

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

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

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

  - Transfer matrix exists



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

MOMENTUM SUBTRACTION

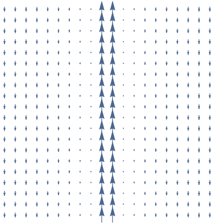
- Removing momentum modes with measure 0 as $V \to \infty$ allowed
- Remove $k = 0$ from momentum sum (QED_{TL})
  - Realised by a constraint term in the action

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

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

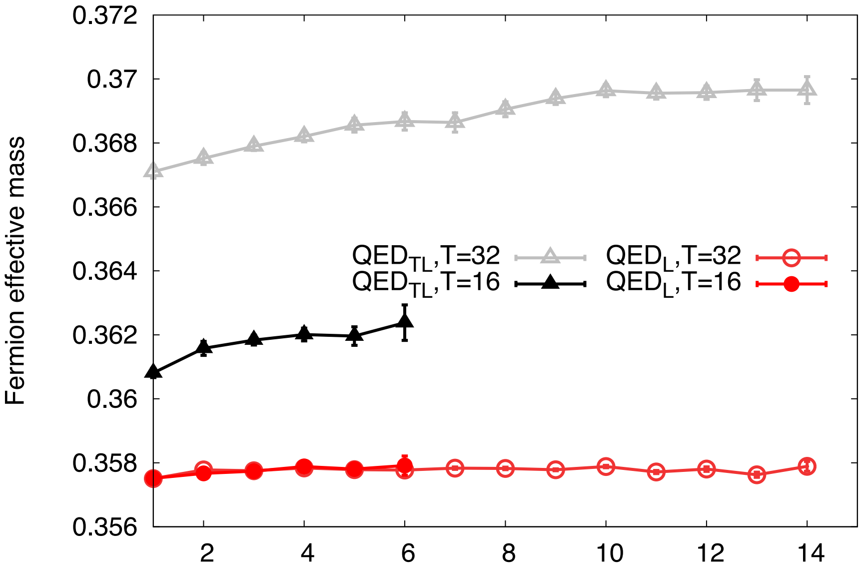
$$\lim_{\xi(t) \to 0} \int dt \frac{1}{\xi(t)} \left(\int d^3 x A_\mu(x) \right)^2$$

  - Transfer matrix exists



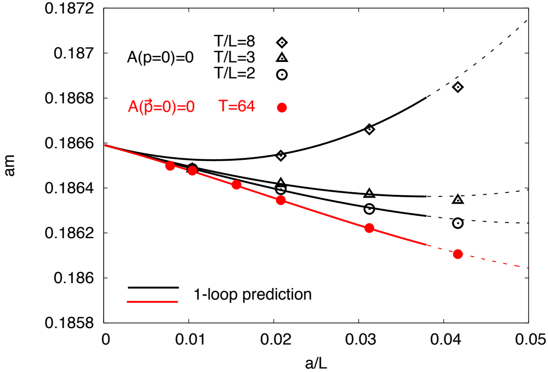
- Gauge fields unaffected in QED_{TL}, only Polyakov loops

QUENCHED QED FV EFFECTS



FINITE VOLUME SUBTRACTION

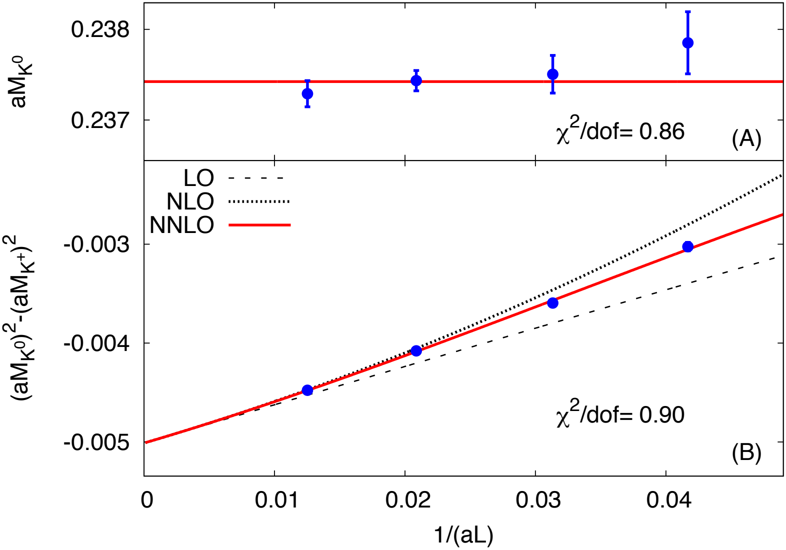
- Universal to $O(1/L^2)$
- Compositmess at $1/L^3$
- Fit $O(1/L^3)$
- Divergent T dependence for $p = 0$ mode subtraction
- No T dependence for $\vec{p} = 0$ mode subtraction



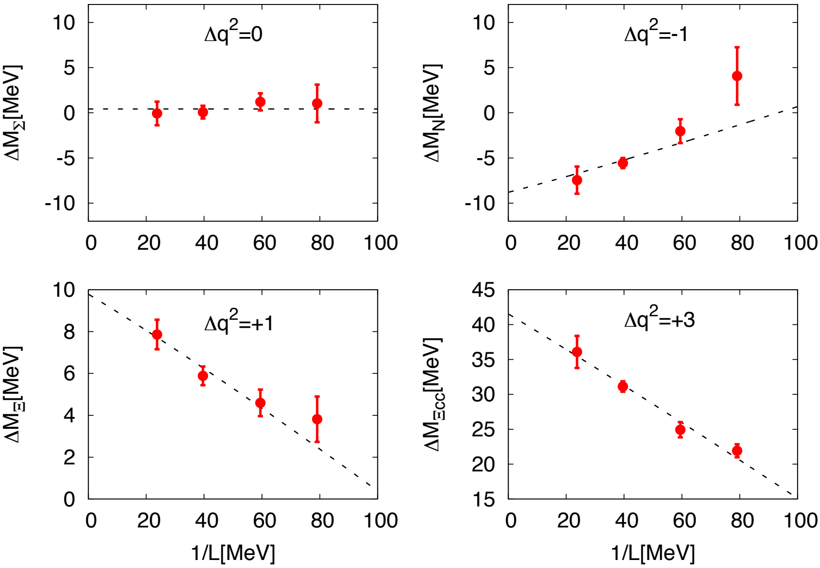
$$\delta m = q^2\alpha\left(\frac{\kappa}{2mL}\left(1+\frac{2}{mL}-\frac{3\pi}{(mL)^3}\right)\right)$$

(BMWc, 2014)

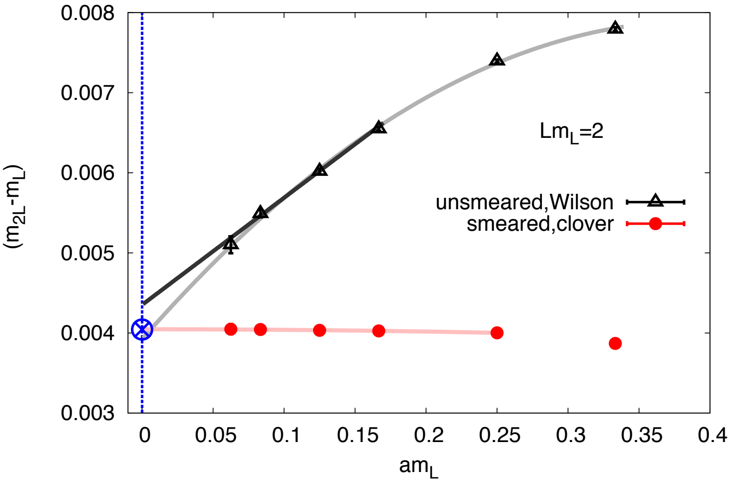
KAON FV IN QCD+QED



BARYON FV IN QCD+QED



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

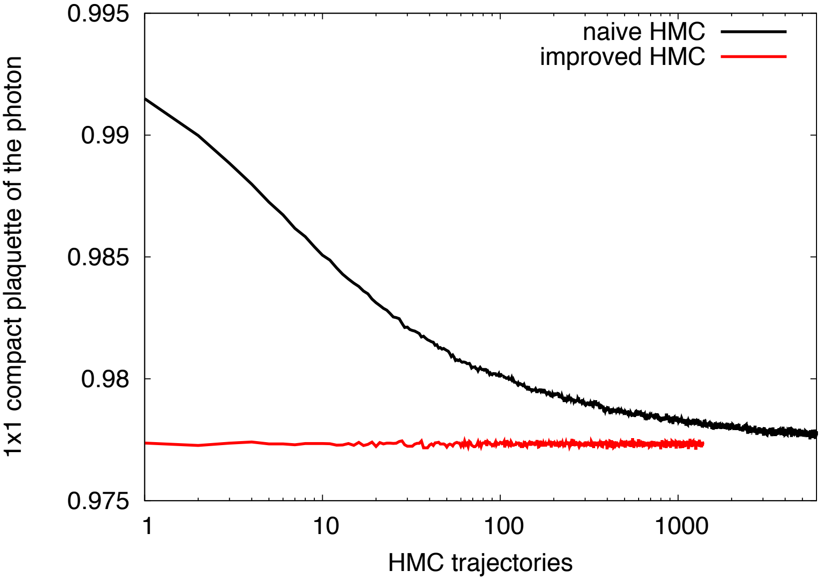
$$\mathcal{H} = \frac{1}{2V_4} \sum_{\mu,k} \left(|\hat{k}|^2 |A_\mu^k|^2 + \frac{|\Pi_\mu^k|^2}{m_k} \right)$$

- Use different masses per momentum

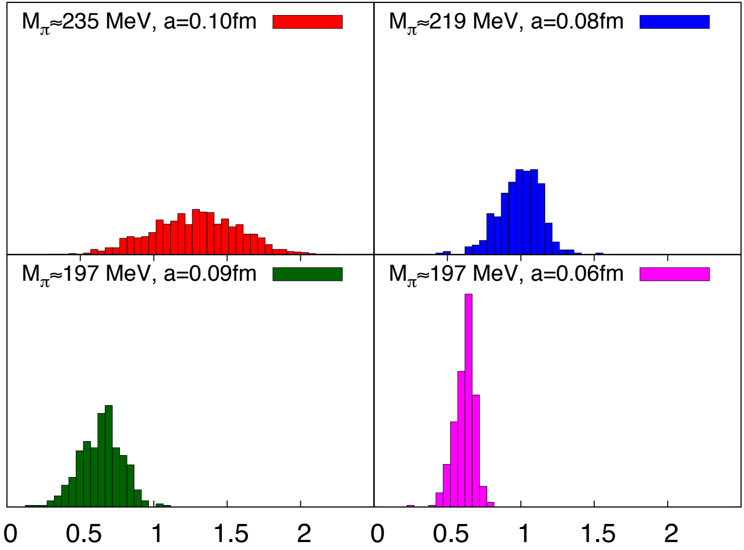
$$m_k = \frac{4|\hat{k}|^2}{\pi^2}$$

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

HMC FOR PHOTON FIELDS



NO EXCEPTIONAL CONFIGURATIONS



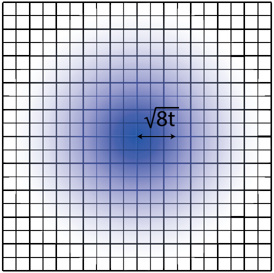
IDENTIFYING THE PHYSICAL POINT

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

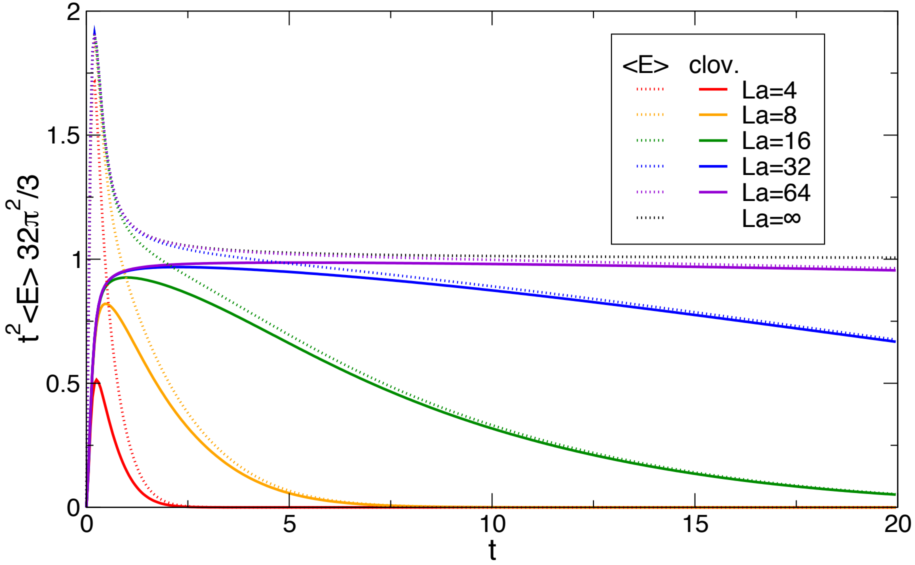
- Requires fixing 5 dimensionless ratios from 6 lattice observables
- 4 "canonical" lattice observables: $M_{\pi^\pm}$, M_{K^+}, M_Ω, M_D
- Strong isospin splitting from $M_{K^\pm} - M_{K^0}$
- what about α?
  - ✗ From $M_{\pi^\pm} - M_{\pi^0}$ ➛ disconnected diagrams, very noisy
  - ✗ From e^- e^- scattering ➛ 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

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

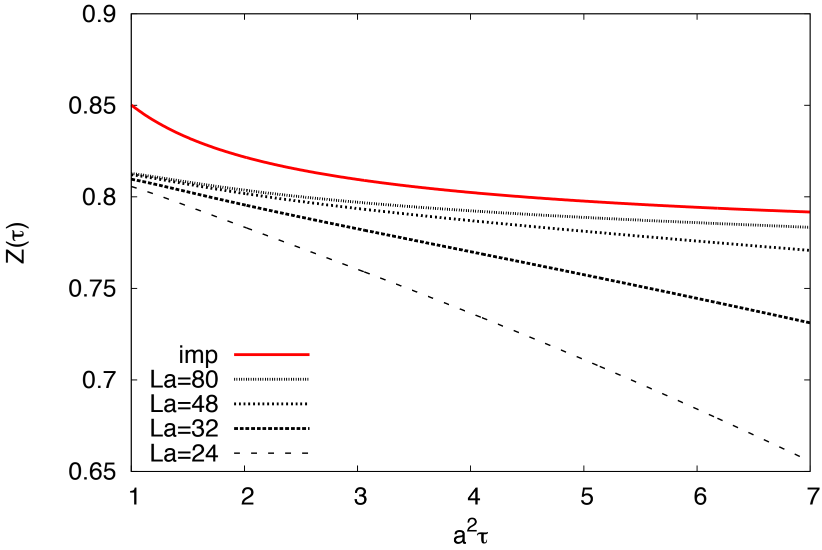
Slightly more complicated for clover plaquette



TREE LEVEL CORRECTION



EFFECT OF TREE LEVEL CORRECTION



SCALING IN RENORMALISED COUPLING

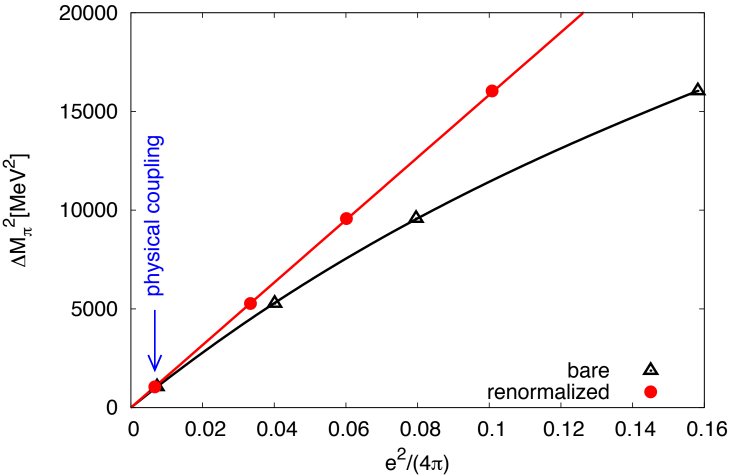
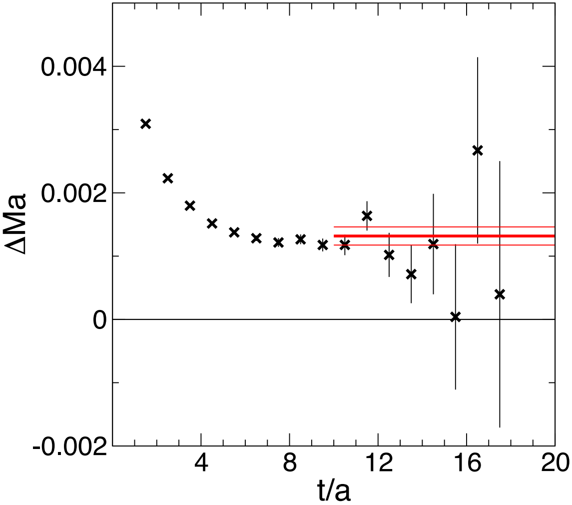


Illustration with precise $\Delta M_\pi^2 = M_{\bar{u}d}^2 - (M_{\bar{u}u}^2 + M_{\bar{d}d}^2)/2$

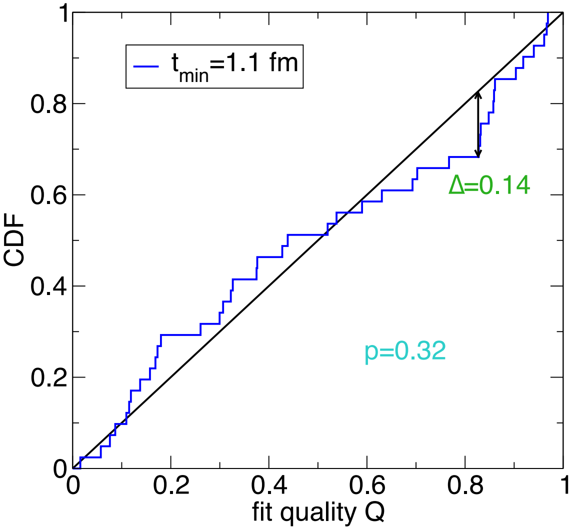
PLATEAUX



- 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



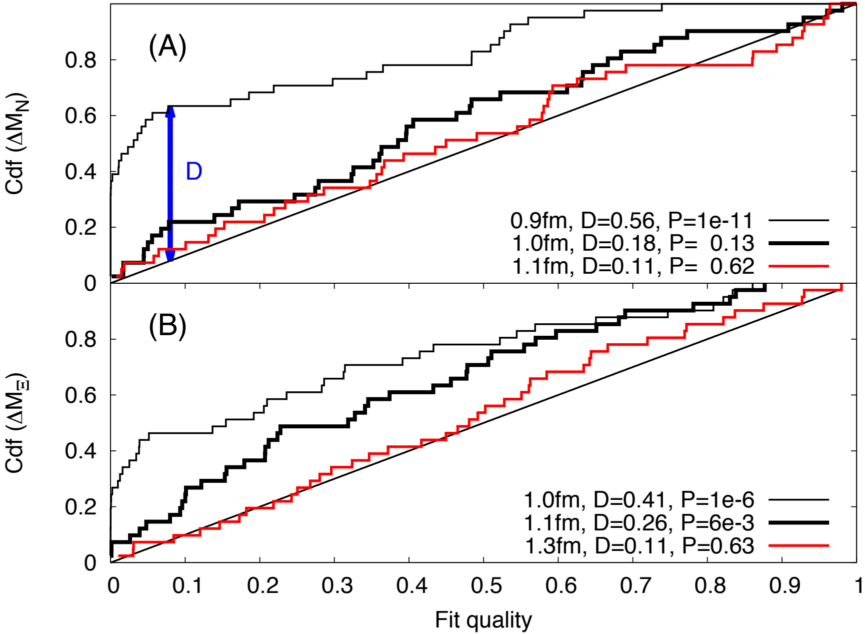
- Need many ensembles
- Plot CDF
- KS test flat distribution

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

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

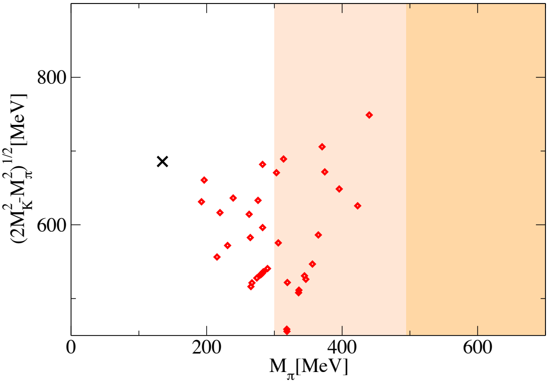
with

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



(A)
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 0.1 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
Fit quality

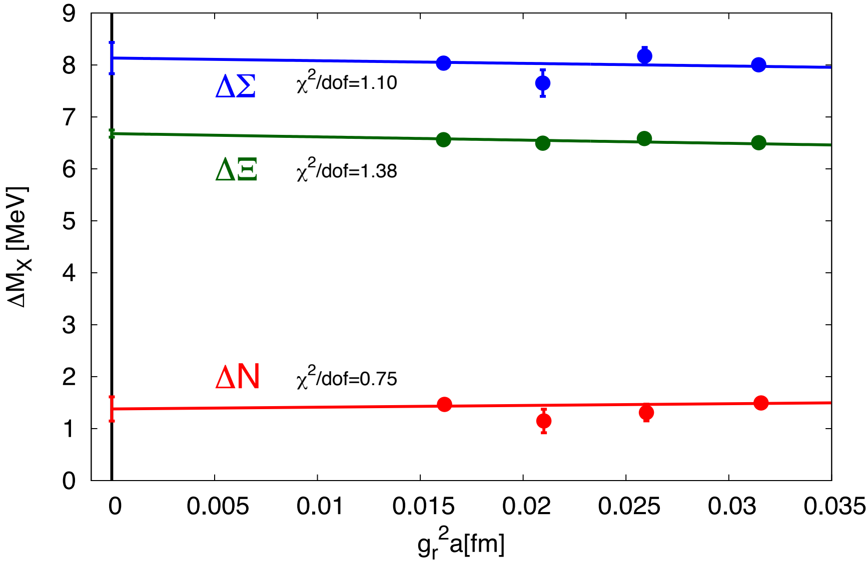
LANDSCAPE



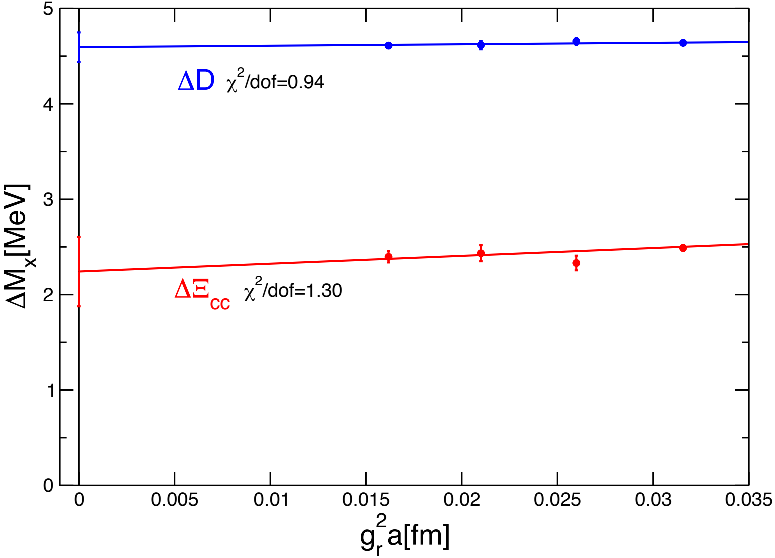
- Small extrapolation to physical point
- Charm mass is physical
- $u - d$ splitting is physical
- Why use $\alpha \gg \alpha^{\text{phys}}$?

- 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

SCALING

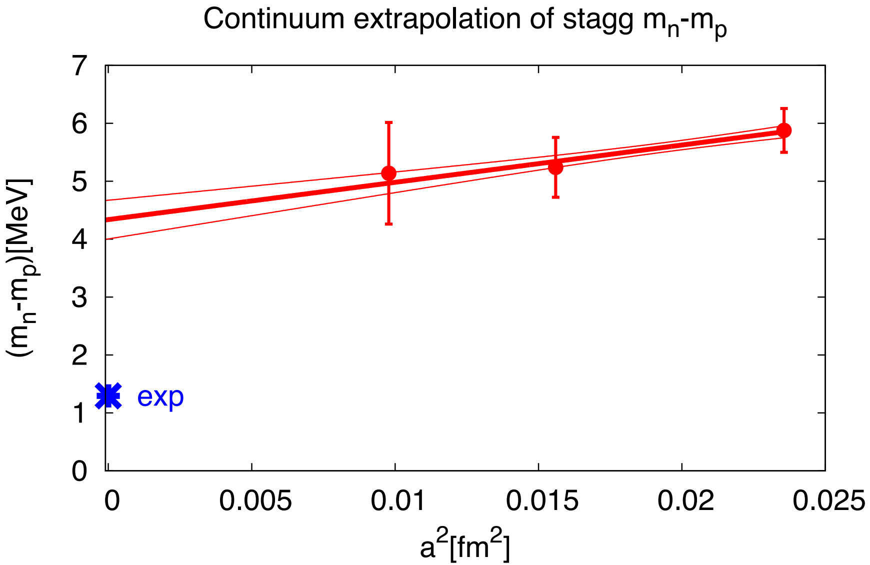

ΔΣ
χ^2/dof=1.10
ΔΞ
χ^2/dof=1.38
ΔN
χ^2/dof=0.75
ΔM_X [MeV]
$g_r^2 a$[fm]
9
8
7
6
5
4
3
2
1
0
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035

SCALING



5
4
3
2
1
0
ΔM_x[MeV]
0
0.005
0.01
0.015
0.02
0.025
0.03
0.035
g_r^2 a[fm]
ΔD χ^2/dof=0.94
ΔΞ_cc χ^2/dof=1.30

DONT DO THIS STAGGERED



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
  - M_π, M_K, M_D, ΔM_K^2 and α interpolations
  - Higher order FV effects
  - Continuum extrapolation

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)

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

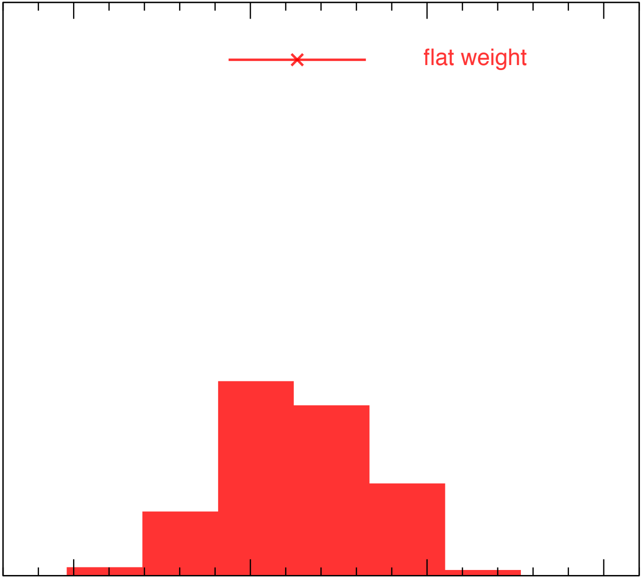
- For $N \to \infty$ and f close to g:

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

where p_m is the number of fit parameters

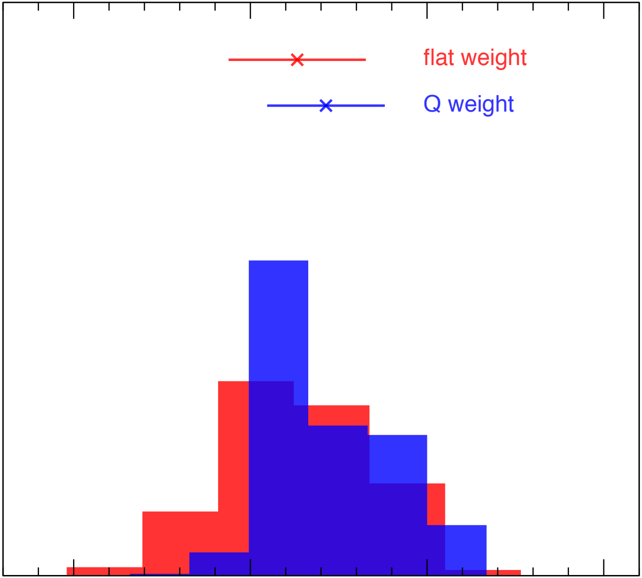
Is this the only correct method?

COMBINING RESULTS



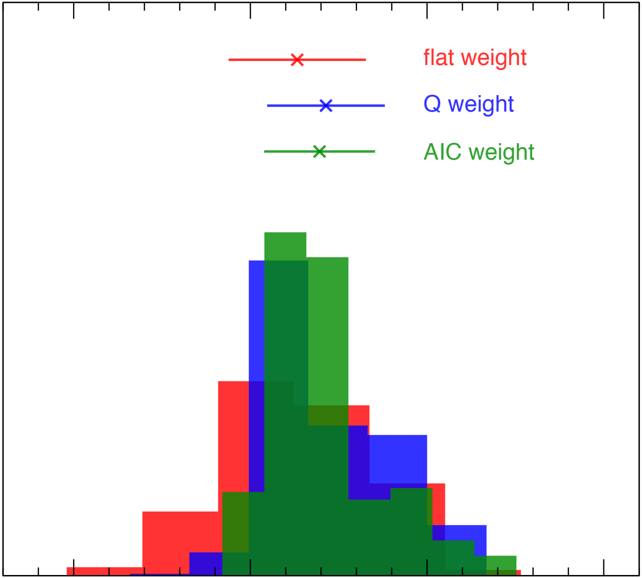
- AIC suppresses strongly
- Other weights more conservative
- Agreement is excellent crosscheck

COMBINING RESULTS



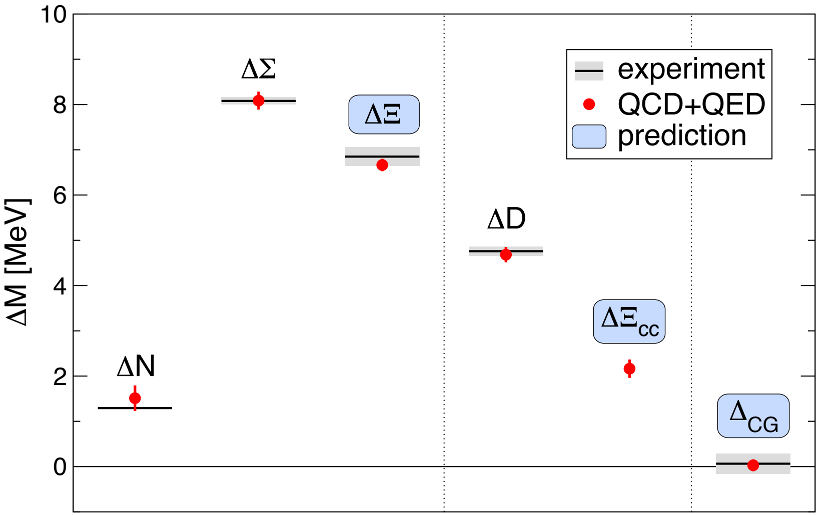
- AIC suppresses strongly
- Other weights more conservative
- Agreement is excellent crosscheck

COMBINING RESULTS



- AIC suppresses strongly
- Other weights more conservative
- Agreement is excellent crosscheck

ISOSPIN SPLITTING

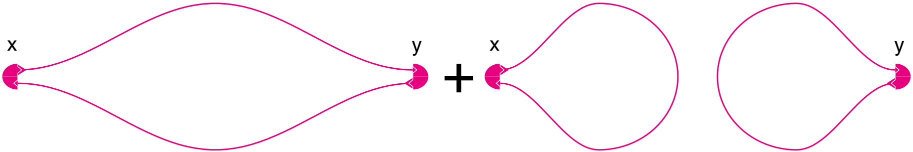


(BMWc 2014)

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

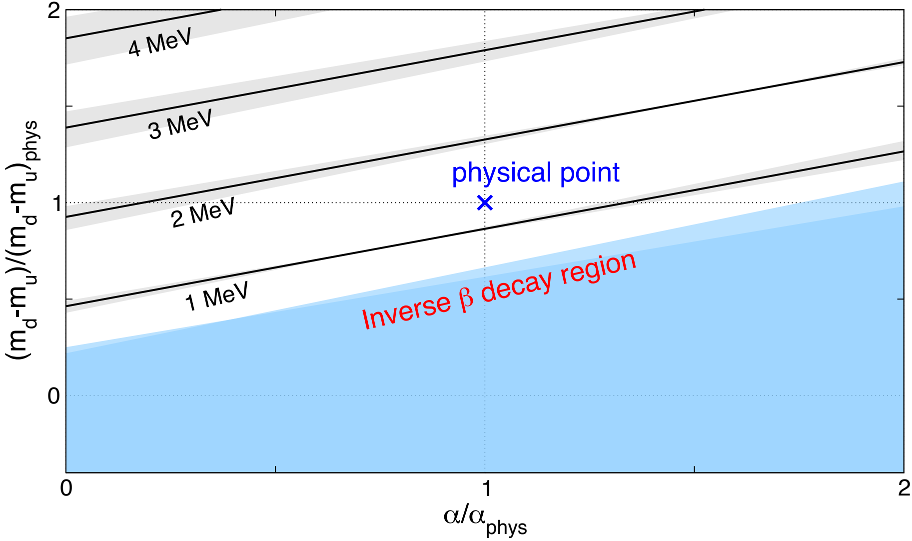
- Quark model relation predicts Δ_{CG} to be small

  (Coleman, Glashow, 1961; Zweig 1964)

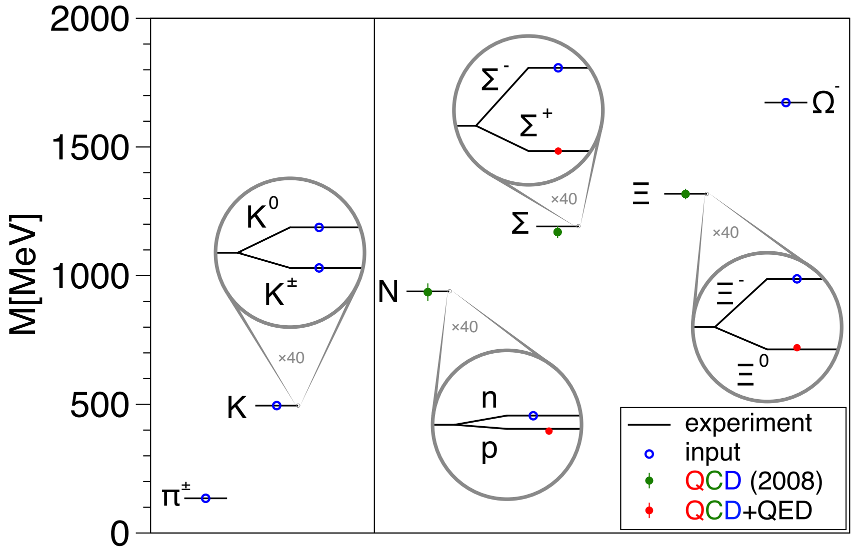
$$\Delta_{\mathrm{CG}} = M(udd) + M(uus) + M(dss) - M(uud) - M(dds) - M(uss)$$

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

NUCLEON SPLITTING QCD AND QED PARTS



PROGRESS



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