Quark mass determinations from BMW collaboration

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Determination of the Fundamental Parameters in QCD
ICTP-SAIFR, Oct. 1st, 2019
How to compute quark masses?

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

Basic recipe:
- Solve QCD for various quark masses

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

- 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 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
Physical point from hadron spectrum

Budapest-Marseille-Wuppertal collaboration

(BMWc, 2008)
In this talk:

- **Computing** $m_{ud}$, $m_s$ in QCD, Wilson type quarks
  - Action and ensembles
  - RI-MOM renormalization, nonperturbative running
  - Ratio-difference method of quark mass extraction
  - Physical point extrapolation and systematic errors

- **Splitting** $\delta m = m_u - m_d$ in QCD+QED, Wilson type quarks
  - QED on the lattice
  - Finite volume effects
  - Physical point extrapolation and systematic errors

- **Precision determination of** $m_s/m_{ud}$ in QCD, staggered quarks
  - Motivation for staggered
  - Action and ensembles
  - Extraction techniques
  - Physical point extrapolation and systematic errors
Our ensembles

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

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

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

\[
\frac{Z_{s, \text{nonpert}}(\mu^2)}{Z_{s, 4\text{-loop}}^{RI}(\mu^2)}
\]

\(\mu = 4 \text{GeV}\)

\(\beta = 3.8\)
Nonperturbative running

- Contact with PT only for finest lattice spacings
- Match different $\beta$ onto each other for low $\mu$, finite $m_r$

- Match at finite $m_r$
- Extract $Z_s$ ratios and iterate matching
- Extrapolate $m_r \to 0$ at high $\mu$
Optional conversion to $\overline{\text{MS}}$

(Ceyrink 1997; Vermaseren, Larin, van Ritbergen, 1997)
Quark mass definitions

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

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

- $m^{\text{ren}}_s = \frac{1}{Z_s} \frac{r_d}{r-1}$

- $m^{\text{PCAC}}$ from
  
  $m^{\text{PCAC}} = \frac{Z_A}{Z_P} m^{\text{PCAC}}$ with
  
  $r = \frac{m^{\text{PCAC}}_s}{m^{\text{PCAC}}_{ud}}$
  
  $r^{\text{ren}} = r$
  
  and reconstruct

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

- 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)

Better use
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 $\frac{M_X(L) - M_X}{M_X} = c M_\pi^{1/2} L^{-3/2} e^{M_\pi L}$ (Colangelo et al., 2005)

![Graph](image-url)
Landscape $L$ vs. $M_\pi$
Continuum limit
Continuum limit

\[ \frac{R_I}{m_{ud}} \text{ (4 GeV)} \] [MeV]

\( \alpha a \) [fm]

- \( a = 0.06 \) fm
- \( a = 0.08 \) fm
- \( a = 0.10 \) fm
- \( a = 0.12 \) fm

Christian Hoelbling (Wuppertal)  Proton neutron mass difference  Oct. 1\textsuperscript{st}, 2019
Continuum limit

\[ m_s / m_{ud} \text{ vs } \alpha a \text{[fm]} \]

- \( a = 0.06 \text{ fm} \)
- \( a = 0.08 \text{ fm} \)
- \( a = 0.10 \text{ fm} \)
- \( a = 0.12 \text{ fm} \)
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

- Perform $O(10000)$ analyses
- Difference: higher order effects
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  - Crosscheck agreement
Systematic error

- Flat weight
- Q weight
- AIC weight

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

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

### Relative contribution to total error:

<table>
<thead>
<tr>
<th></th>
<th>stat.</th>
<th>plateau</th>
<th>scale</th>
<th>mass</th>
<th>renorm.</th>
<th>cont.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_s$</td>
<td>0.702</td>
<td>0.148</td>
<td>0.004</td>
<td>0.064</td>
<td>0.061</td>
<td>0.691</td>
</tr>
<tr>
<td>$m_{ud}$</td>
<td>0.620</td>
<td>0.259</td>
<td>0.027</td>
<td>0.125</td>
<td>0.063</td>
<td>0.727</td>
</tr>
<tr>
<td>$m_s/m_{ud}$</td>
<td>0.921</td>
<td>0.200</td>
<td>0.078</td>
<td>0.125</td>
<td>—</td>
<td>0.301</td>
</tr>
</tbody>
</table>

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

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

with \( j_\mu = \bar{q} Q \gamma_\mu q \)

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

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

**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)
- $\pi^+$, $\rho$, 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

\[ S_{\text{QED}} = \frac{1}{2V_4} \sum_{\mu,k} |\hat{k}|^2 |A^{k}_{\mu}|^2 \quad \text{with} \quad \hat{k}_{\mu} = \frac{e^{ia k_{\mu}} - 1}{ia} \]

- Momentum modes decouple \(\Rightarrow\) quenched theory trivial
Finite volume gauge symmetry

- Periodicity requirement from gauge field

\[ A_\mu(x) \rightarrow A_\mu(x) + \frac{1}{e} \partial_\mu \Lambda(x) \implies \partial_\mu \Lambda(x) = \partial_\mu \Lambda(x + L) \]

- is loser than from fermion field

\[ \psi(x) \rightarrow e^{-i\Lambda(x)} \psi(x), \quad \bar{\psi}(x) \rightarrow \psi(x)e^{i\Lambda(x)} \implies \Lambda(x) = \Lambda(x + L) \]

- 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

\[ \mathcal{L}_{\text{src}} = J_\mu \bar{\psi}\gamma^\mu \psi \quad J_\mu \rightarrow J_\mu - ic_\mu \]
QED in finite volume

- Gauge invariant definition of no external source:
  \[ \frac{e}{V_4} \int d^4 x A_\mu(x) + iJ_\mu = 0 \]

  with partial gauge fixing \( J_\mu = 0 \) \( \Rightarrow \) QED\(_\text{TL} \)

- Imposing electric flux neutrality per timeslice:
  \[ \frac{e}{V_3} \int d^3 x A_i(t, \bar{x}) = 0 \]

  with partial gauge fixing \( A_0(t, \bar{p} = 0) = 0 \) \( \Rightarrow \) QED\(_\text{L} \)
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 \( \implies \) 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
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Quenched QED FV effects

Fermion effective mass

\( m_u \) and \( m_d \) in QCD+QED  QED in finite volume

\( \text{QED}_{TL, T=32} \)
\( \text{QED}_{L, T=32} \)
\( \text{QED}_{TL, T=16} \)
\( \text{QED}_{L, T=16} \)
Finite volume subtraction

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

\[ \Delta M \text{ [MeV]} \]

- \( \Delta \Sigma \)
- \( \Delta \Xi \)
- \( \Delta D \)
- \( \Delta \Xi_{cc} \)
- \( \Delta N \)
- \( \Delta_{CG} \)

Experiment
- QCD+QED
- Prediction

(BMWc 2014)
Masses of the $u$ and $d'$ quarks

Goal:
- Directly compute $m_u$ and $m_d$

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

Computing $m_u - m_d$:
- Parameterize $\delta m = m_u - m_d$ via $\Delta M^2 = M_{uu}^2 - M_{dd}^2$
  \[
  \Delta M^2 = 2B_2 \delta m + O(m_{ud} \alpha, m_{ud} \delta m, \alpha^2, \alpha \delta m, \delta m^2)
  \]
- Power counting: $O(\delta m) = O(m_{ud})$
- Condensate parameter $B_{2}^{\overline{MS}}(2\text{GeV}) = 2.85(7)(2)\text{GeV}$ (BMWc 2013)
Our dataset

![Graph showing $M_{dd}$ vs $M_{uu}$ in MeV$^2$. The graph features markers for different datasets: physical, physical $\delta m$, mass isospin $m_u = m_d$, and intermediate. Shaded regions represent the physical $\frac{m_u}{m_d}$ and $\delta m$ regions. The mass isospin line $m_u = m_d$ is also marked.]
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

\[ \Delta_{\text{QED}} M_K^2 \text{ [MeV]} \]

- \( a = 0.11 \text{ fm} \)
- \( a = 0.09 \text{ fm} \)
- \( a = 0.07 \text{ fm} \)
- \( a = 0.06 \text{ fm} \)
- \( a = 0.05 \text{ fm} \)
Chiral interpolation

\[ \Delta_{\text{QED}} M^2_K \]

\[ (M^2_{\pi^+})_{\text{ph}} \]

\[ M^2_{\pi^+} \text{ [MeV}^2\text{]} \]

\[ a = 0.11 \text{ fm} \]

\[ a = 0.09 \text{ fm} \]

\[ a = 0.07 \text{ fm} \]

\[ a = 0.06 \text{ fm} \]

\[ a = 0.05 \text{ fm} \]
Results

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

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

(BMWc, 2016)
Motivation

Why staggered?

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

Meson mass extraction

$N_f = 2 + 1 + 1$

staggered ensembles

4 stout smeared

\[ \frac{M_K^2}{M_K^{2(\phi)}} - \frac{1}{2} M_{\pi}^2 \]

\[ \frac{M_K^2(\phi)}{M_K^{2(\phi)}} - \frac{1}{2} M_{\pi}^2(\phi) \]

\[ \beta = 3.8400 (7) \]

\[ \beta = 3.9200 (2) \]

\[ \beta = 4.0126 (3) \]
Meson mass extraction

Extracting staggered meson masses:
  • Multi-state fit
  • Time-shifted propagator

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

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

define time shifted propagator

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

Determine \( \Delta \) by minimizing effective mass fluctuations
  • Cross-checked with variational multi-state fit
Meson mass extraction
Meson mass extraction
Physical point interpolation
Continuum extrapolation

The graph shows the ratio $m_{ud}/m_s$ as a function of $a^2 [fm^2]$. The data points are marked with flags indicating the FLAG 2+1+1 scheme.
Systematic error

- 64 variations of analysis:
  - 2 plateaux ranges
  - 4 $m_s$ continuum terms
  - 4 $m_{ud}$ continuum terms
  - 2 $\chi$ interpolation mixing

Other variations crosschecked: no further relevant terms found

Final result:

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

![Graph showing the ratio of quark masses $m_u/m_d$ and $m_s/m_{ud}$ with data points and error bars. The graph includes contributions from various collaborations such as FLAG (2019), MILC, BMW, and PDG.]

- FLAG average for $N_f=2+1+1$:
  - MILC 18
  - MILC 17
  - RM123 17
  - ETM 14

- FLAG average for $N_f=2+1$:
  - BMW 16
  - MILC 16
  - QCDSF/UKQCD 15
  - PACS-CS 12
  - Laiho 11
  - BMW 10A, 10B
  - Blum 10
  - MILC 09A
  - MILC 09
  - MILC 04, HPQCD/MILC/UKQCD 04

- Phenomenology (PDG):
  - Oller 07
  - Narison 06
  - Kaiser 98
  - Leutwyler 96
  - Weinberg 77

- Other contributions:
  - RBC/UKQCD 14B
  - RBC/UKQCD 12
  - PACS-CS 12
  - Laiho 11
  - BMW 10A, 10B
  - RBC/UKQCD 10A
  - Blum 10
  - PACS-CS 09
  - MILC 09A
  - MILC 09
  - PACS-CS 08
  - RBC/UKQCD 08
  - MILC 04, HPQCD/MILC/UKQCD 04

Oct. 1st, 2019
BACKUP
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
- 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

![Graph showing the stability of different forces over time. The graph illustrates various forces such as Gauge force, RHMC force, Pf0 force, Pf1 force, Pf2 force, Pf3 force, and Pf4 force. The x-axis represents time in units of k (kilograms), ranging from 2k to 10k, and the y-axis shows the magnitude of the forces. Each force is represented by a different colored line, indicating their stability over the period of interest.]
No exceptional configs

Inverse iteration count (1000/N\textsubscript{cg})

- $\beta=3.31$, $M_\pi \approx 135$ MeV
- $\beta=3.61$, $M_\pi \approx 120$ MeV
- $\beta=3.5$, $M_\pi \approx 130$ MeV
- $\beta=3.7$, $M_\pi \approx 180$ MeV
- $\beta=3.8$, $M_\pi \approx 220$ MeV
Topological sector sampling

Topological charge $\beta=3.8$, $m_{ud}=-0.02$, $m_s=0$

worst case
Autocorrelation time (finest lattice, small mass)

\[ \tau_{\text{int}} = 27.3(7.4) \]

(MATLAB code from Wolff, 2004-7)

Normalized autocorrelation for $lq_{\text{ren}}$ at $\beta=3.8$, $m_{ud}=-0.02$, $m_s=0$

With statistical errors for $lq_{\text{ren}}$ at $\beta=3.8$, $m_{ud}=-0.02$, $m_s=0$
Chiral continuum fit

![Graph showing the relationship between $M$ (GeV) and $M_{\pi}^2$ (GeV$^2$)].

- $\Omega$: Dotted line, $a \approx 0.125$ fm
- $N$: Dashed line, $a \approx 0.085$ fm
- $a \approx 0.065$ fm: Solid line

Physical $M_{\pi}$
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
- $M_p + M_{e^-} \geq M_n$
- No hydrogen
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Is the fine structure relevant?

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- $m_u < m_d$: $M_p < M_n$
- $m_u = m_d$: $M_p > M_n$
  - Proton decays
- $M_p + M_{e^-} \gtrsim M_n$
  - No hydrogen
Is the fine structure relevant?

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

Neutron
Big bang nucleosynthesis

$M_n - M_p$ determines deuterium bottleneck

(Burles, Nollett, Turner, 1999)
Hydrogen abundance

(Bernstein, Brown, Feinberg, 1989)
The light up quark

1\textsuperscript{st} generation: \( m_u < m_d \)  

2\textsuperscript{nd} generation: \( m_c > m_s \)  

3\textsuperscript{rd} generation: \( m_t > m_b \)
Tiny finite volume effects

- FV effects tiny
- Dedicated FV run
- Perfect agreement with FV $\chi$PT (Colangelo et al. 2005)

$M_\pi L=3$, $M_\pi L=4$

ignored in final analysis

$aM_\pi$ vs $L/a$
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

\[ \Delta q^2 = 0 \]

\[ \Delta M_{\Sigma}^{\pm} \text{[MeV]} \]

\[ 0 \quad 20 \quad 40 \quad 60 \quad 80 \quad 100 \]

\[ \Delta M_{\Lambda} \text{[MeV]} \]

\[ 0 \quad 20 \quad 40 \quad 60 \quad 80 \quad 100 \]

\[ \Delta q^2 = -1 \]

\[ \Delta M_{\Xi}^{\pm} \text{[MeV]} \]

\[ 0 \quad 20 \quad 40 \quad 60 \quad 80 \quad 100 \]

\[ \Delta M_{\Xi^c} \text{[MeV]} \]

\[ 0 \quad 20 \quad 40 \quad 60 \quad 80 \quad 100 \]

\[ \Delta q^2 = +1 \]

\[ \Delta q^2 = +3 \]
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 \( \alpha \)?
  - \( \times \) From \( M_{\pi^\pm} - M_{\pi^0} \Rightarrow \) disconnected diagrams, very noisy
  - \( \times \) From \( e^- e^- \) scattering \( \Rightarrow \) far too low energy
  - \( \times \) From \( M_{\Sigma^+} - M_{\Sigma^-} \Rightarrow \) baryon has inferior precision
  - \( \checkmark \) Take renormalized \( \alpha \) as input directly
  - \( \Rightarrow \) Use the QED gradient flow
    Analytic tree level correction

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

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

\[ p(x) = \sum_{j} \frac{(-1)^{j-1}2}{e^{-2j^2x^2}} \]
Scaling

\[ \Delta \Sigma \quad \chi^2/\text{dof}=1.10 \]

\[ \Delta \Xi \quad \chi^2/\text{dof}=1.38 \]

\[ \Delta N \quad \chi^2/\text{dof}=0.75 \]
Scaling

\[ \Delta D \quad \chi^2 / \text{dof} = 0.94 \]

\[ \Delta \Xi_{cc} \quad \chi^2 / \text{dof} = 1.30 \]

\[ \Delta M_X \quad \text{[MeV]} \]

\[ g_r^2 a \quad \text{[fm]} \]
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

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

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

(Coleman, Glashow, 1961; Zweig 1964)

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

\[
\Delta_{CG} \propto ((m_d - m_u)(m_s - m_u)(m_s - m_d), \alpha(m_s - m_d))
\]
Nucleon splitting QCD and QED parts

The graph shows the mass differences between the proton and neutron, denoted as $(m_d - m_u)_{phys}$, plotted against the ratio $\alpha/\alpha_{phys}$. The horizontal lines represent different energy levels in MeV: 4 MeV, 3 MeV, 2 MeV, and 1 MeV. The physical point is marked by a cross. The shaded area indicates the inverse $\beta$ decay region.
Resulting initial hydrogen abundance
PROGRESS

MASS DIFFERENCES  QCD and QED contributions

![Diagram showing mass differences and contributions](image)

- Experiment
- Input
- QCD (2008)
- QCD + QED

Christian Hoelbling (Wuppertal)

Proton neutron mass difference

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Locality properties

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

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

6-stout case:

\[ \| \partial D(x,y)/\partial U_\mu(x+y) \| \]

\[ |z|/a \]

\[ a \approx 0.125 \text{ fm} \]
\[ a \approx 0.085 \text{ fm} \]
\[ a \approx 0.065 \text{ fm} \]
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 ($r_\chi$ resp. $M_\chi$)
  - $O(a)$ 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 $\rightarrow$ final result
  - Central 68% $\rightarrow$ systematic error

- Statistical error from bootstrap of the medians
Prediction from CKM unitarity ($|V_{us}|/|V_{ud}|$)

- $N_f = 2+1+1$
  - ETM '10
  - NPLQCD '06
  - HPQCD/UKQCD '07
  - MILC '10
  - ALV '08

- $N_f = 2+1$
  - RBC/UKQCD '10
  - PACS-CS '09

- $N_f = 2+1$
  - THIS WORK
  - QCDSF-UKQCD '10
  - JLQCD/TWQCD '09

$\frac{f_K}{f_\pi}$
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 $\eta \rightarrow \pi\pi\pi$
    
  $Q^2 = \frac{1}{2} \left( \frac{m_s}{m_{ud}} \right)^2 \frac{m_d - m_u}{m_{ud}}$

  ✓ Transform precise $m_s/m_{ud}$ into $(m_d - m_u)/m_{ud}$

  - We use the conservative $Q = 22.3(8)$ (Leutwyler, 2009)
Comparison

\[ m_{ud} \]

\[ m_s \]

MeV

MeV

2 3 4 5 6

2 3 4 5 6

PACS-CS 09
HPOCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPOCD 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 09
Maltman 01

PDG 09

BMWe 10

PACS-CS 09
HPOCD 09
MILC 09A
MILC 09
PACS-CS 08
RBC/UKQCD 08
CP-PACS 07
MILC 07
HPOCD 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

BMWe 10
Chiral cuts

![Graph showing the ratio of masses as a function of minimal pion mass. The x-axis represents minimal \( m_\pi \) in MeV, ranging from 120 to 240. The y-axis represents the ratio \( m_s/m_{ud} \), ranging from 25 to 30. There are data points at minimal pion masses of 120, 200, and 240 with corresponding error bars.](image-url)
Moderate smearing (1 stout) improves scaling dramatically
Updating photon field

Long range QED interaction ➞ huge autocorrelation in standard HMC

- Solution: HMC in momentum space

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

- 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

1x1 compact plaquette of the photon vs. HMC trajectories

- naive HMC
- improved HMC
TREE LEVEL CORRECTION

\[ t^2 \frac{<E>}{32\pi^2/3} \]

- \(<E>\) clov.
- La=4
- La=8
- La=16
- La=32
- La=64
- La=\infty

Graph showing the behavior of \( t^2 \frac{<E>}{32\pi^2/3} \) as a function of \( t \).
EFFECT OF TREE LEVEL CORRECTION

\[ Z(\tau) \]

\[ a^2 \tau \]

- imp
- La=80
- La=48
- La=32
- La=24
SCALING IN RENORMALISED COUPLING

Illustration with precise $\Delta M_{\pi}^2 = M_{ud}^2 - (M_{uu}^2 + M_{dd}^2)/2$
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

- $N$ measurements $\Gamma_i$ 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 $g$:

$$J_m = -\frac{\chi^2_m}{2} - p_m$$

where $p_m$ is the number of fit parameters

Is this the only correct method?