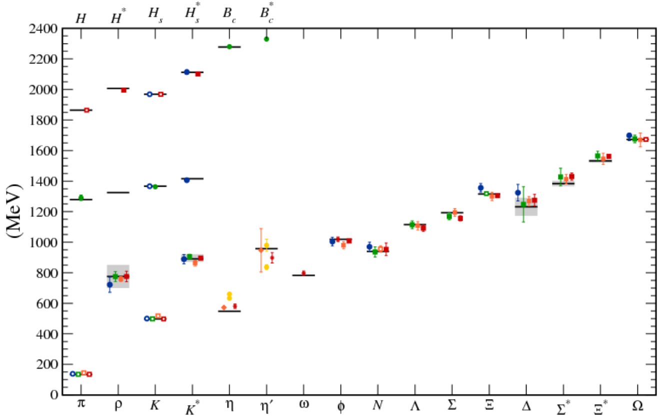
The neutron-proton mass difference

Kalman Szabo
Forschungszentrum Jülich - Universität Wuppertal

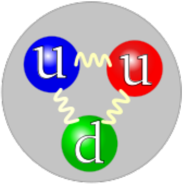
Budapest-Marseille-Wuppertal collaboration:
S. Durr, Z. Fodor, C. Hoelbling, S. Katz, S. Krieg, L. Lellouch,
T. Lippert, A. Portelli, B. Toth

Hadron spectrum

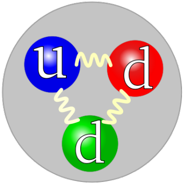
Several lattice QCD groups calculated the nucleon mass (and many more) to a few % accuracy. Compilation by [Kronfeld '13]:



Proton

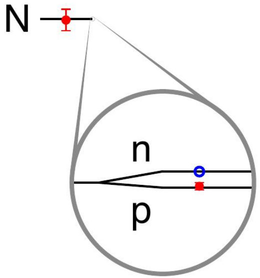


Neutron



SU(2) isospin symmetry: u$\leftrightarrow$d

Isospin symmetry



SU(2) is violated by
- quark mass difference
- electric charge difference

On the per mil level $\Delta M_N / M_N = 0.14\%$ arising from a competition of the two.

The value of ΔM_N is **neccesary for the observed Universe:**

- $\delta M_N < 0.05\% \rightarrow$ inverse β-decay leaves only neutrons
- $\delta M_N > 0.14\% \rightarrow$ much faster β-decay, no heavy elements

Calculating ΔM_N?

Lattice QCD already **reached a few percent** precision on several observables (hadron spectrum, quark masses, decay constants, matrix elements, hadron vacuum polarization, . . .).

Reaching a better precision requires the implementation of isospin symmetry violation.

The **very first thing** is to check if ΔM_N comes out correctly.

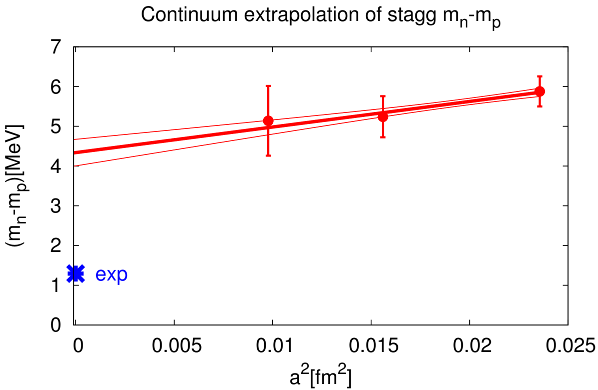
Fine structure of the spectrum

arXiv:1406:4088

At dawn of lattice calculations (early 80's):

"It is difficult to get a grossly incorrect hadron spectrum."

$m_n - m_p$ with staggered fermions



QCD is wrong? No. Staggered is wrong? No.

Problem with naive staggered proton operator.

In the continuum staggered symmetry group there are two different proton (uud) states differing in the taste structure. They have different masses, if $m_u \neq m_d$. The naive operator on the lattice couples to both. It can be challenging to separate the two states (need multiple operators).

Novelties

First full dynamical calculation of QCD+QED with non-degenerate u, d, s, c quarks.

All systematics on $m_n - m_p$ are taken into account upto $\mathcal{O}(\alpha^2)$.

Addressed **several issues in QED:**

- zero-mode subtraction
- finite volume corrections
- large noise/signal
- large autocorrelation

Challenging: **unprecedented precision** is required (x1000 more statistics for $m_n - m_p$ than for m_N)

Zero-mode subtraction

$$A_\mu(k=0)$$

Zero-mode of photon field is troublesome:

- in finite volume perturbative calculations are not well defined

$$\frac{\alpha}{V}\sum_k \frac{1}{k^2}\ldots \longrightarrow \text{contains a straight } 1/0\ !$$

- HMC algorithm is ineffective in updating the zero mode

Removing zero mode does not change infinite volume physics.

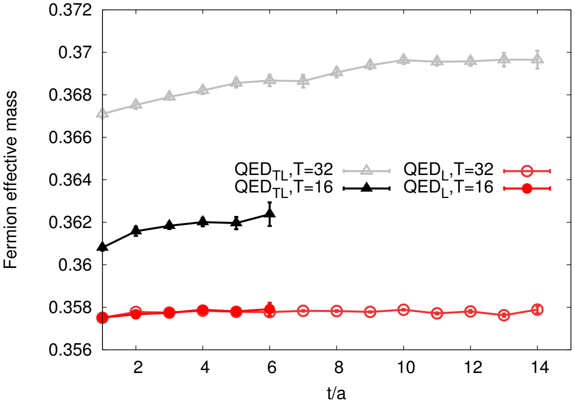
Many possible schemes, we study two choices:

- **QED_TL**: $A_\mu(k=0)=0$ [Duncan et al '96]
- **QED_L**: $A_\mu(k_0,\vec{k}=0)=0$ for all k_0 [Hayakawa,Uno '08]

Zero-mode subtraction

In **QED_TL masses are ill-defined** (used in previous studies).

No clear mass-plateaus, mass increases with T. It violates reflection positivity!



QED_L does not have these problems, T independent masses.

Issues with QED

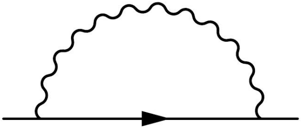
- **zero-mode subtraction**
- **finite volume corrections**
- **dynamical QED: noise/signal**
- **dynamical QED: autocorrelation**

Finite-volume effects in pure QED

Instead of the usual exponential [Luscher 85], the FV effects are **power like** $(L^{-1}, L^{-2}, \dots)$. The FV effects are **large**, comparable to ΔM_N.

In pure QED can be studied by calculating:

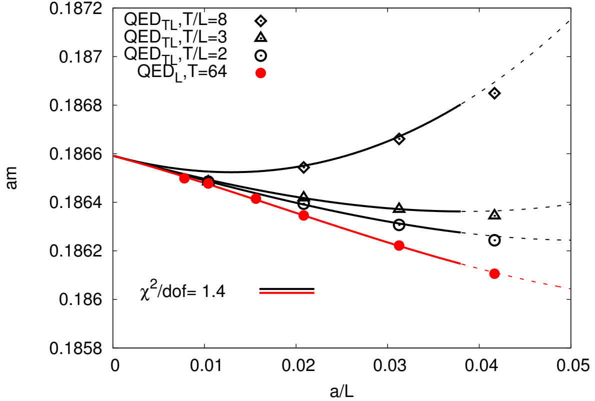
$$\int \frac{dk_0}{(2\pi)} \left(\int \frac{d^3k}{(2\pi)^3} - \frac{1}{L^3} \sum_{\vec{k} \neq 0} \right) \quad \times$$



Power like FV effects arise from photon travelling around the lattice $(k \rightarrow 0)$.

Finite-volume effects in pure QED

Analytical result (line) is used to verify the numerical code (point). Perfect agreement.



The different zero-mode subtraction schemes give the same infinite volume result.

Finite volume effects in general

Proton is a **composite particle**, what are the FV effects?

- mesons in SU(3) PQ χ-PT [Hayakawa,Uno '08]
- meson/baryons in non-rel. eff. field theory [Davoudi,Savage '14]
- point particle in QED [BMWc '14]

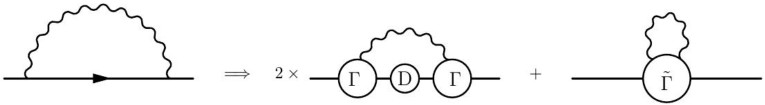
$\rightarrow$ same $1/L$ and $1/L^2$ behaviour

$$m(T,L)/m = 1 - \frac{\alpha \cdot 1.418...}{(mL)} - \frac{\alpha \cdot 2.837...}{(mL)^2} + \mathcal{O}\left(\frac{\alpha}{L^3}\right)$$

The $1/L$ is a purely classical effect (static charge in a box).

Finite volume effects in general

Point particle propagator/vertex is replaced by dressed propagator and vertices (3pt and 4pt):



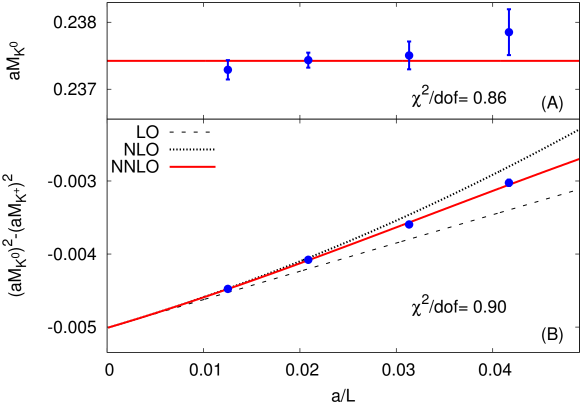
Use Ward's identities, Lorentz structure, expand Feynman-integrands in k, argue as in [Luscher 85]:

→ universal $1/L$ and $1/L^2$ behaviour

Large FV effects can be removed analytically.

FV dependence of the kaon mass

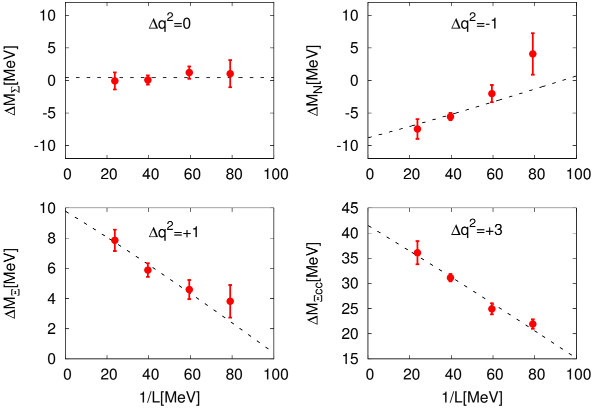
dedicated FV study: L=2.5...8.0 fm at the same parameters



Neutral kaon shows no volume dependence.
Kaon splitting is perfectly described by formula with fitted $1/L^3$.

FV dependence of baryon masses

dedicated FV study: L=2.5...8.0 fm at the same parameters



Σ splitting shows no volume dependence (cancels).
analysis strategy: include analytic corrections for the two universal orders and fit coefficient of $1/L^3$ (almost always insignificant)

Issues with QED

- **zero-mode subtraction**
- **finite volume corrections**
- **dynamical QED: noise/signal**
- **dynamical QED: autocorrelation**

Dynamical QED

We are concerned with the QED interaction of quarks. An isospin splitting can be calculated as:

$$\langle \Delta \rangle_e = \int [dA][dU] \; \exp(-\mathbf{S}_\gamma[\mathbf{A}] + S_g[U]) \cdot \det D[\mathbf{eA}, U] \cdot \Delta[\mathbf{eA}, U]$$

Electro-quenched approximation

$$\det D[eA, U] \to \det D[0, U]$$

Used in most previous studies on isospin splittings.

Probably small error (SU3 suppressed), but it is still $\mathcal{O}(e^2)$, so it has to be eliminated in a full calculation.

Dynamical QED eliminates this error. How to do?

Dynamical QED

Generate **gluon+photon** configurations simultaneously with a dynamical algorithm.

But there is a **noise/signal problem**:

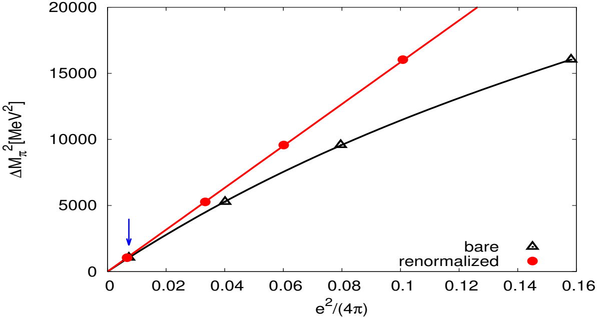
$$\langle \Delta \rangle_e = e \cdot \text{noise} + e^2 \cdot \text{signal} + \dots$$

Simulate at **larger than physical** α, so signal outweighs noise:

$$\frac{e^2}{4\pi} = \frac{1}{137} \longrightarrow \frac{1}{10}$$

Dynamical QED

data shows significant deviation from linear as the function e^2



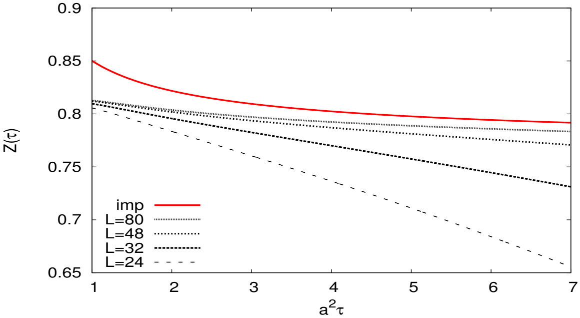
expansion in couplings at the energy scale of the process converge much faster: **define a coupling at a hadronic scale** (e_R^2)

simulate $\begin{cases} \text{neutral ensembles } e = 0 \\ \text{charged ensembles } e^2 \sim 4\pi/10 \end{cases}$ + linear interpolation in e_R^2

Dynamical QED

we use the **Wilson-flow to define the renormalized charge**

$$e_R^2(\tau)/e^2 = Z(\tau) = \tau^2 \langle F_{\mu\nu}^{(A)} F_{\mu\nu}^{(A)}(\tau) \rangle$$



there is sizeable finite volume dependence, that can be removed by tree-level improvement

eventually we want Thomson-limit $\tau \to \infty$, in practice we read off at $\sqrt{8\tau} \sim 0.5$fm, difference is small

Issues with QED

- **zero-mode subtraction**
- **finite volume corrections**
- **dynamical QED: noise/signal**
- **dynamical QED: autocorrelation**

Dynamical QED

long range QED → **huge autocorrelation in standard HMC**
problem is already present in the free case (uncoupled oscillators):

$$\mathcal{H} = \frac{1}{V}\sum_{k,\mu} \frac{P_{k,\mu}^2}{2} + \frac{k^2 A_{k,\mu}^2}{2}$$

small k oscillators are practically unchanged after a unit trajectory
Solution: update small/large k modes using a long/short trajectory length, achieved by **changing kinetic term in HMC dynamics**

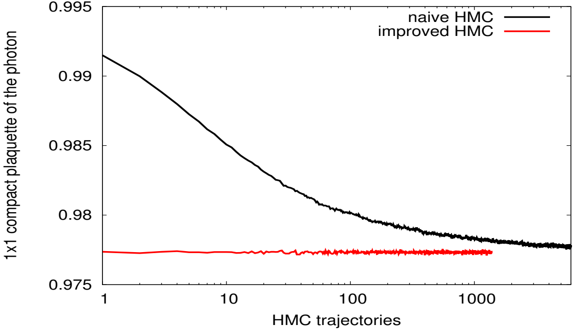
$$\mathcal{H} = \frac{1}{V}\sum_{k,\mu} \frac{P_{k,\mu}^2}{2M_k} + \frac{k^2 A_{k,\mu}^2}{2} \quad \text{with} \quad M_k = 4k^2/\pi^2$$

all modes forget initial condition after a unit trajectory
⇒ **improved HMC has no autocorrelation** in the free case

Dynamical QED

$$\mathcal{H} = \frac{1}{V} \sum_{k,\mu} \frac{P_{k,\mu}^2 \pi^2}{4k^2} + \frac{k^2 A_{k,\mu}^2}{2}$$

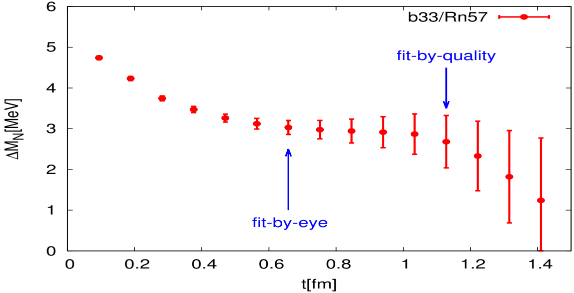
only works with zero mode subtraction (like QED_TL or QED_L)



requires an FFT in every HMC step in the interacting case

Extracting the masses

Which timeslices are appropriate to extract the mass? If t too small, excited states contaminate. If t too large, signal gets lost.



Choosing the plateau by eye gives too small errors, and the result is in disagreement with the experimental ΔM_N.

Look at the distribution of fit-qualities over the 41 ensembles. Choose such a fit range, that Q has a uniform distribution.

$\Rightarrow t_{min} = 1.1$ **fm for the neutron-proton mass difference**

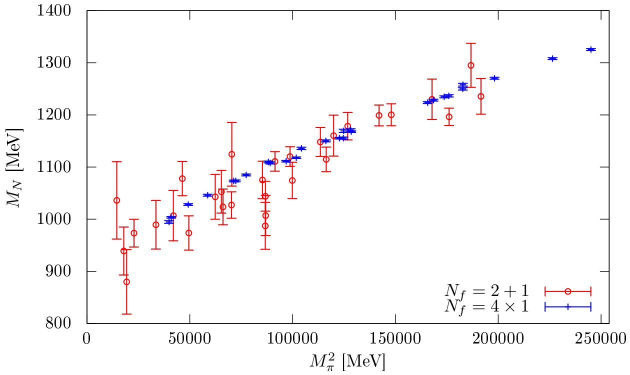
Sketch of simulations

- four lattice spacings $a = 0.102 \ldots 0.064$ fm (insensitive)
- pion masses $M_\pi = 195 \ldots 490$ MeV (insensitive)
- 27 neutral ensembles with $m_u \neq m_d$
- 14 charged ensembles including
  - finite volume scan $L = 2.4 \ldots 8.2$ fm
  - electric charge scan $e = 0 \ldots 1.41$
- parameter tuning with QCDSF strategy $m_u + m_d + m_s$ const
- $\mathcal{O}(10k)$ trajectory long ensembles, $\mathcal{O}(500)$ source positions on each configuration using 2-level multigrid inverter [Frommer et al '13] and variance reduction technique [Blum,Izubuchi,Shintani '13]

Simulations

Abount 1000× more statistics for ΔM_N [BMWc '14] than for M_N [BMWc '08]. Recent algorithmic improvements:

- using 2-level multigrid inverter [Frommer et al '13]
- variance reduction technique [Blum,Izubuchi,Shintani '13]



Sketch of analysis

- mass splittings on 41 ensembles are modelled by functions like

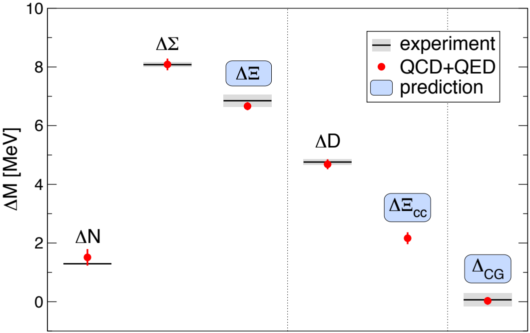
$$\Delta M_X = F_X(\pi^+, K^0, D^0) \cdot \alpha + G_X(\pi^+, K^0, D^0) \cdot \Delta M_K^2$$

- physical point is defined by the inputs: π^+, K^0, K^+, D^0 and α, scale is set by Ω mass
- separating QED and QCD contributions to isospin splittings
- **systematic error estimation**:
  - carrying out several equally plausible fits differing in functional form of F_X/G_X
  - weight different models by **Akaike's information criterion**: prefers fits with lower χ^2 values, but punishes with too many fit parameters

$$AIC = \chi^2 + 2 \cdot \#\text{parameters}$$

  - systematic error is the width of the weighted histogram

Final results

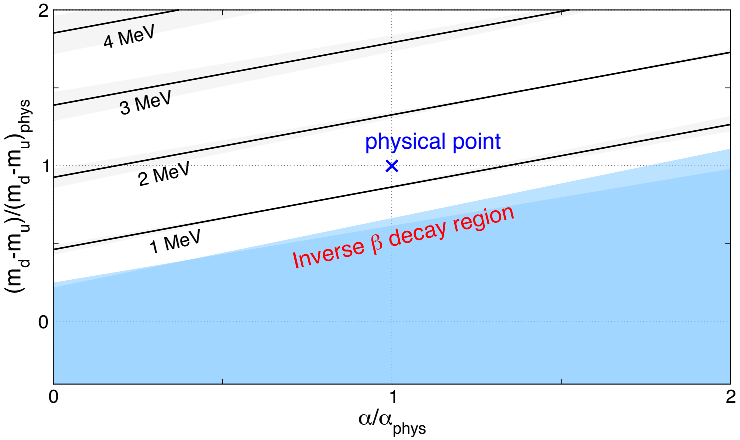


arXiv:1406:4088

- 5σ signal for neutron-proton mass difference
- three predictions + calculation of QCD/QED contributions
- $\Delta_{CG} = \Delta M_N - \Delta M_\Sigma + \Delta M_\Xi$ (Coleman-Glashow relation)
- full calculation - all systematics are estimated

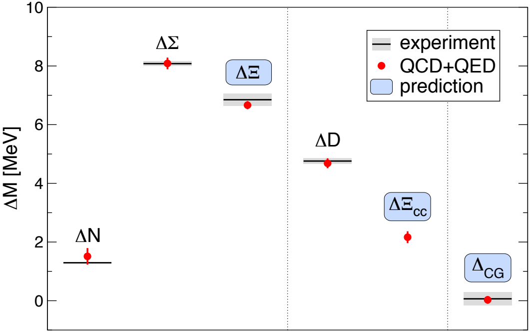
Could things have been different?

How changing α and $m_d - m_u$ changes ΔM_N?



Outlook for the (far) future: How does our own existence constrain the parameters of the Standard Model?

Final results



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