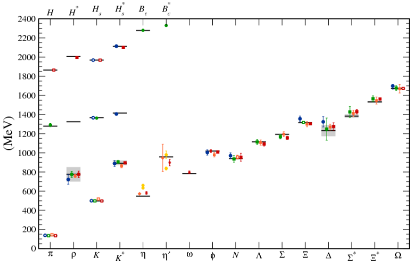
The neutron-proton mass difference

Kalman Szabo
Forschungszentrum Jülich - Universität Wuppertal

Budapest-Marseille-Wuppertal collaboration

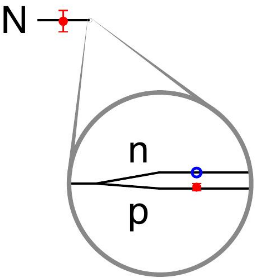
Hadron spectrum

[Kronfeld '13]



several lattice QCD groups calculated the nucleon mass (and many more) to a few % accuracy

SU(2) isospin symmetry: u↔d



SU(2) is violated by

- quark mass difference
- electric charge difference

on the per mil level $\Delta M_N / M_N = 0.14\%$

$\Rightarrow$ **Can we calculate it?**

Fine structure of the spectrum

arXiv:1406:4088

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

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

- 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]

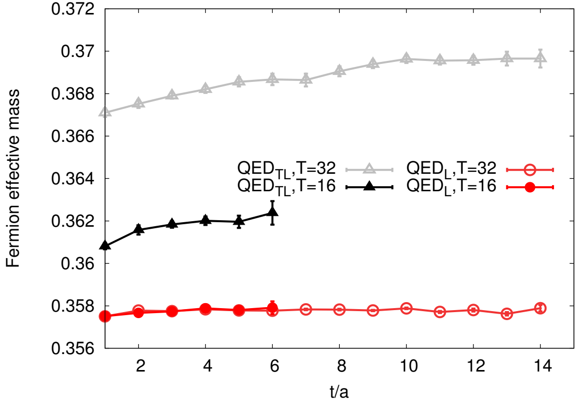
Zero-mode subtraction

Most previous studies used QED_TL.

It violates reflection positivity!

$\rightarrow$ no clear mass plateux $\rightarrow$ mass increases with T

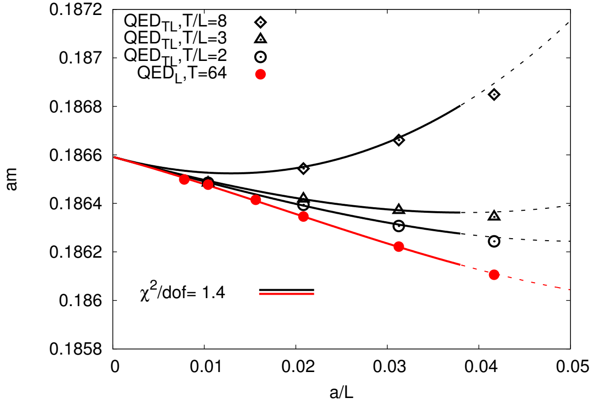
Numerical study in pure QED:



QED_L does not have this problem, T independent masses.

Finite volume effects in pure QED

The different schemes give the same infinite volume result.



FV effects are power like $(1/L, 1/L^2, \ldots)$

Finite volume effects in general

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

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

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

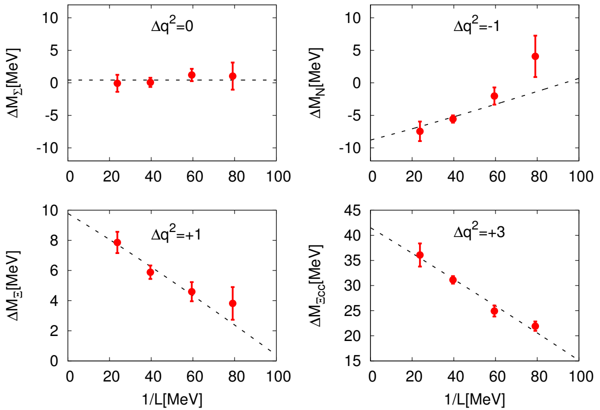
$$m(T,L)/m = 1 - q^2\alpha\frac{\kappa}{2mL}\left[1+\frac{2}{mL}\right] + \mathcal{O}\left(\frac{\alpha}{L^3}\right)$$

holds in a general field theory (using Ward's identities [BMWc '14])

large FV effects can be removed analytically

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)

Dynamical QED

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

$$\langle \Delta \rangle_e = \int [dA][dU] \ \exp(-S_\gamma[A] + S_g[U]) \det D[eA, U] \Delta[eA, U]$$

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

Two strategies:

1. **reweight $e = 0$ gluon+free photon configurations**

$$\langle \Delta \rangle_e = \left\langle \Delta \frac{\det D(e)}{\det D(0)} \right\rangle_0$$

$\rightarrow$ exponentially expensive in the volume, needs sophisticated techniques to estimate the det D ratio

[Aoki et al '12][Ishikawa et al '12]

2. **generate gluon+photon configurations** with the correct weight

$\rightarrow$ no issue with going to large volumes

$\rightarrow$ there is a **noise/signal problem**:

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

Simulate at larger than physical couplings, where signal outweighs noise. [QCDSF '13][BMWc '14]

Dynamical QED

long range QED $\rightarrow$ **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**

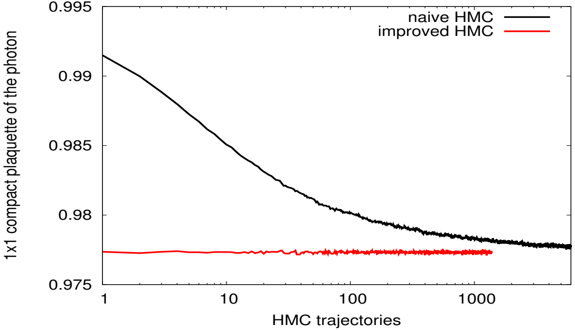
$$\mathcal{H} = \frac{1}{V} \sum_{k,\mu} \frac{P_{k,\mu}^2}{2M_k} + \frac{k^2 A_{k,\mu}^2}{2} \quad \text{with} \quad M_k = 4k^2/\pi^2$$

all modes forget initial condition after a unit trajectory
$\Rightarrow$ **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

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]

Sketch of analysis

- mass splittings on 41 ensembles are modelled by functions like

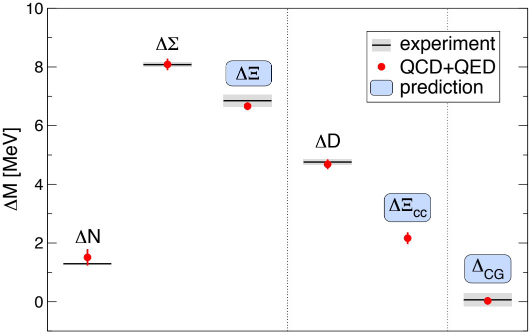
$$\Delta M_X = F_X(\pi^+, K^0, D^0) \cdot \alpha + G_X(\pi^+, K^0, D^0) \cdot \Delta M_K^2$$

- to get the results at the physical point set $\pi^+, K^0, D^0, \Delta M_K^2$ and α to their physical values; 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