Ab-initio calculation of the neutron-proton mass difference

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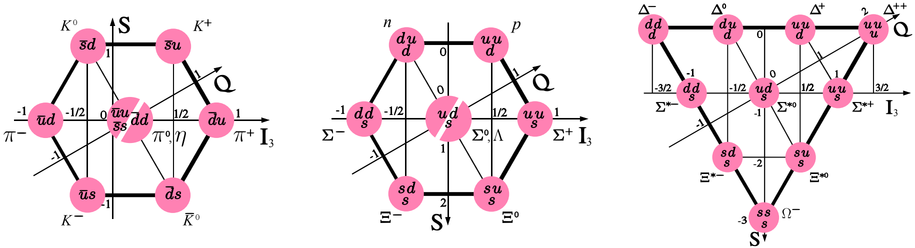
Budapest-Marseille-Wuppertal collaboration (BMWc)

(arXiv:1406.4088)



Particles along horizontal lines have particularly similar properties

Result of near $SU(2)$ isospin symmetry of strong interaction (Heisenberg '32), which we know today acts on

$$\begin{pmatrix} u \\ d \end{pmatrix} \longrightarrow \exp[i\vec{\theta}\cdot\vec{\tau}] \begin{pmatrix} u \\ d \end{pmatrix}$$

Only broken by small, often competing

$$3\,\frac{m_d - m_u}{M_N} \sim 1\% \qquad \text{and} \qquad (Q_u - Q_d)^2\,\alpha \sim 1\%$$

Motivation: isospin symmetry breaking

Small but hugely important . . . and challenging

- $M_n - M_P \gtrsim m_e + m_{\nu_e}$ → stability of $^1\mathrm{H}$ and ordinary matter
  But: $2\frac{M_n - M_p}{M_p + M_n} \sim 0.14\%$ → Big Bang nucleosynthesis
  → existence & properties of nuclides
- EM is limiting factor in knowledge of m_u and m_d (e.g. FLAG 13)
  → though very unlikely (e.g. FLAG 13), if $m_u = 0$ → solution to strong CP problem
  → But: $m_u/M_p \sim 0.002$
- Important flavor observables are becoming very precisely known: e.g. $\mathrm{err}(m_{ud}), \mathrm{err}(m_s) \sim 2\%$, $\mathrm{err}(m_s/m_{ud}) \lesssim 1\%$, $\mathrm{err}(F_K) \sim 1\%$, $\mathrm{err}(F_K/F_\pi) \sim 0.5\%$, $\mathrm{err}(F_+^{K\pi}(0)) \sim 0.8\%$
  → isospin breaking corrections required to search for new physics

Can these effects be reliably computed in the fundamental theory?

Can be computed to $O(\alpha, (m_d - m_u))$, but mix with nonperturbative QCD

⇒ **nonperturbative QCD tool**
⇒ **include EM and $m_u \neq m_d$**

QCD+QED challenges

Important challenges addressed:

- formulate QED in a finite box (long-range interactions)
  $\rightarrow$ photon zero-mode subtraction (Hayakawa et al '08, BMWc '14)
- subtract large finite-volume effects ("soft" photons)
  $\rightarrow$ determine coefficients of leading effects analytically (BMWc '14)
- consistently renormalize QCD+QED theory
  $\rightarrow$ renormalize α using Wilson flow (Lüscher '10, BMWc '14)
- avoid unwanted phase transitions of lattice QED
  $\rightarrow$ use non-compact formulation (Duncan et al '96)
- fight large autocorrelations of QED field
  $\rightarrow$ Fourier accelerated algorithm (BMWc '14)
- fight large noise/signal ratio
  $\rightarrow$ larger than physical e (Duncan et al '96)

QCD+QED challenges

- finding asymptotic time-range for hadron mass extractions
  $\rightarrow$ method based on Kolmogorov-Smirnov test (BMWc '14)
- robust estimation of systematic errors
  $\rightarrow$ improve Science '08 method using Akaike information criterion (BMWc '14)
- unprecedented precision required ($\times 1000$ more statistics for ΔM_N than for M_N)
  $\rightarrow$ $O(10k)$ trajectories/ensemble, $O(500)$ sources/configuration, using 2-level multigrid inverter (Frommer et al '13) and variance reduction technique (Blum et al '13)

QCD + QED à la BMWc

Borsanyi et al (BMWc), arXiv:1406.4088

First full QCD + QED calculation w/ non-degenerate u, d, s, c quarks

- 41 large statistics simulations with $m_u \neq m_d$
  $\rightarrow$ 41 m_u, m_d, m_s, m_c combinations w/ pion masses $M_\pi = 195 \nearrow 420\,\mathrm{MeV}$ (sufficient for light hadron masses cf. Science '08)
- 5 values of $e = 0 \nearrow 1.4$ (physical ~ 0.3)
- 4 lattice spacings $a = 0.06 \nearrow 0.10\,\mathrm{fm}$
- 11 volumes w/ $L = 2.1 \nearrow 8.0\,\mathrm{fm}$
- New algorithm for (non-compact) QED
- Highly improved algorithms and codes
- State-of-the-art physics analysis and determination of uncertainties

$\rightarrow$ fully-controlled calculation of per mil, $M_n - M_p$ effect w/ total error $< 20\%$

Finite-volume QED and zero-mode problem

A $T \times L^3$ spacetime with periodic BCs has the topology of a four-torus

On four-torus **zero mode**, $\tilde{A}_\mu(k=0)$, of photon field is troublesome:

- usual perturbative calculations are not well defined

$$\alpha \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2} \cdots \quad \longrightarrow \quad \frac{\alpha}{TL^3} \sum_k \frac{1}{k^2} \cdots$$

$\uparrow$ possible IR divergences but not in physical qties

$\uparrow$ contains a straight 1/0!

- HMC algorithm is ineffective in updating the zero mode

$\Rightarrow$ **remove zero mode(s)**

$\rightarrow$ modification of $\tilde{A}_\mu(k)$ on set of measure zero

$\rightarrow$ does not change infinite-volume physics

Zero-mode subtractions

Extensive analytical and numerical study of:

QED_{TL}: set $\tilde{A}_\mu(k=0)=0$ on $T\times L^3$ four-torus (Duncan et al '96)

- Used in electroquenched studies
- Violates reflection positivity! (BMWc '14)

  $\rightarrow$ no Hamiltonian

  $\rightarrow$ divergences when L fixed, $T\rightarrow\infty$ (BMWc '14)

QED_{L}: set $\tilde{A}_\mu(k_0,\vec{k}=0)=0$ on $T\times L^3$ four-torus for all $k_0=2\pi n_0/T$, $n_0\in\mathbb{Z}$

- Used here (suggested in Hayakawa & Uno '08)
- Satisfies reflection positivity (BMWc '14)

  $\rightarrow$ Coulomb gauge, $\vec{\nabla}\cdot\vec{A}=0$, ensures existence of Hamiltonian (BMWc '14)

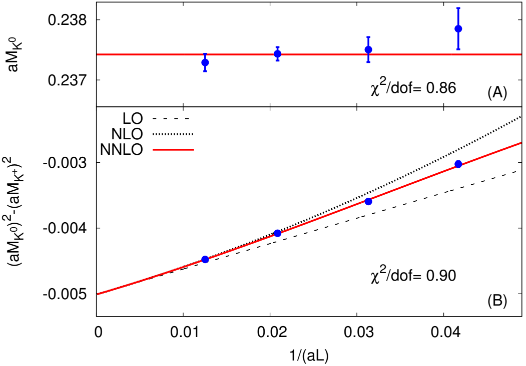
  $\rightarrow$ well defined $T,L\rightarrow\infty$ limit (BMWc '14)

- $1/L$ and $1/L^2$ corrections to masses have known coefficients fixed by **Ward identities**, independent of particle spin and structure (BMWc '14)

  $\rightarrow$ leading FV effects can be removed analytically

FV effects in kaon masses

Dedicated FV study w/ $L = 2.4 \nearrow 8.0\,\mathrm{fm}$ and other parameters fixed (bare $\alpha \sim 1/10$, $M_\pi = 290\,\mathrm{MeV}$, $M_{K^0} = 450\,\mathrm{MeV}$, $a = 0.10\,\mathrm{fm}$)



- M_{K^0} has no significant volume dependence
- $M^2_{K^0} - M^2_{K^+}$ well described by universal $1/L$, $1/L^2$ and fitted $1/L^3$ terms

Sketch of analysis

- Mass splittings on 41 ensembles modeled by

$$\Delta M_X = F_X(M_{\pi^+}, M_{K^0}, M_{D^0}, L, a) \cdot \alpha_{\rm ren} + G_X(M_{\pi^+}, M_{K^0}, M_{D^0}, a) \cdot \Delta M_K^2$$

  - F_X, G_X parametrize m_{ud}, m_s, m_c, , L and a dependences
  - Results at physical point obtained by setting M_{π^+}, M_{K^0},M_{D^0} to their physical values, $L \to \infty$ and $a \to 0$, w/ a determined by M_{Ω^-}

- Systematic error estimation
  - Carry out $O(500)$ equally plausible analyses, differing in time-fit ranges for M_X determinations, functional forms for $F_X, G_X, \ldots$
  - Use Akaike information criterion

$$\text{AIC} = \chi^2_{\rm min} + 2k$$

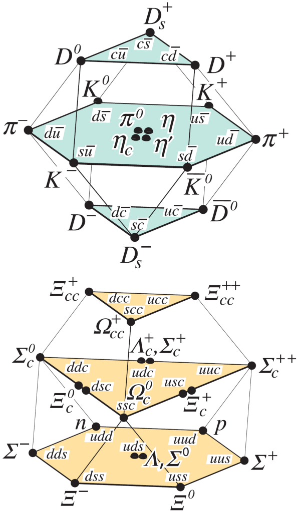
  - Weight different analyses w/

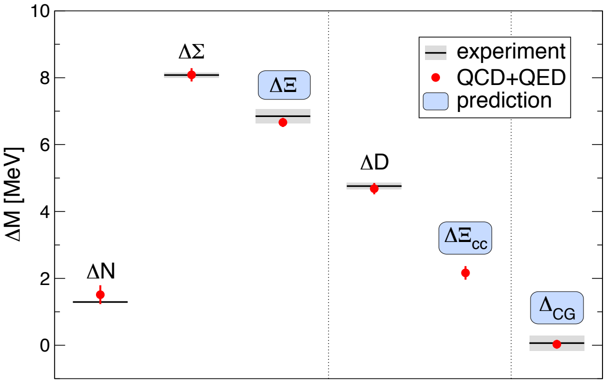
$$\exp\left[-(\text{AIC} - \text{AIC}_{\rm min})/2\right]$$

  - central value = weighted mean, syst. error = (weighted variance)$^{1/2}$
  - Final results with other weights or median and distribution width consistent

- Statistical error from variance of central values from 2000 bootstrap samples

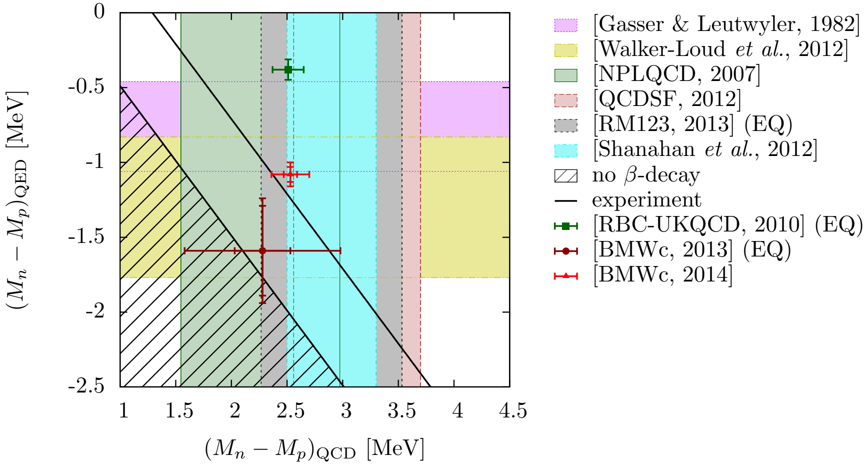
Results for isospin mass splittings





- 5σ signal for $M_n - M_p$
- 3 predictions
- $\Delta_{\mathrm{CG}} = \Delta M_N - \Delta\Sigma + \Delta\Xi = O(\alpha(m_s - m_{ud}), \delta m(m_s - m_{ud})^2)$ (Coleman-Glashow relation)
- Full calculation: all systematics are estimated

Separation of QED and $(m_d - m_u)$ contributions



(From A. Portelli, plenary talk at Lattice 2014)

Conclusions

- Have now a good theoretical understanding of QCD+QED on a finite lattice
- Powerful theorem determines coefficients of leading $1/L$ and $1/L^2$ finite-volume (FV) corrections

  $\Rightarrow$ large QED FV effects can be extrapolated away reliably and precisely
- Have all of the algorithms required to reliably simulate QCD+QED
- Our QCD+QED simulations w/ u, d, s, c sea quarks and $m_u \neq m_d$

  $\rightarrow$ full description low-energy standard model w/ potential precision of $O(\alpha^2, 1/N_c m_b^2) \sim 10^{-3}$

  $\rightarrow$ increase in accuracy $\sim \times 10$ compared to state-of-the-art $N_f = 2+1$ simulations with intrinsic errors of $O(\alpha, \delta m, 1/N_c m_c^2) \sim 10^{-2}$
- Isosplittings in hadron spectrum determined accurately w/ full control over uncertainties
- Determine nucleon splitting as 5σ effect

Outlook

- Fully controlled computation of the u & d quark masses
- Isospin corrections to hadronic matrix elements (e.g. K_{ℓ_2}, K_{ℓ_3}, $K \to \pi\pi, \ldots$)

  $\to$ bring indirect search for new physics to new level
- QCD+QED to compute hadronic corrections to anomalous magnetic moment of the μ, $(g_\mu - 2)$

  $\to$ currently $> 3\sigma$ deviation between SM and experiment w/ $\sim$matched errors

  $\to$ need to bring SM calculation to new level in view of new experiments $\gtrsim 2017$ that will reduce error by 4
- ...

Progess since 2008