Ab-initio calculation of the neutron-proton mass difference

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(based mainly on arXiv:1406.4088, PRL 111 '13, Science 322 '08)

Nucleon mass difference

Well known experimentally (PDG '13)

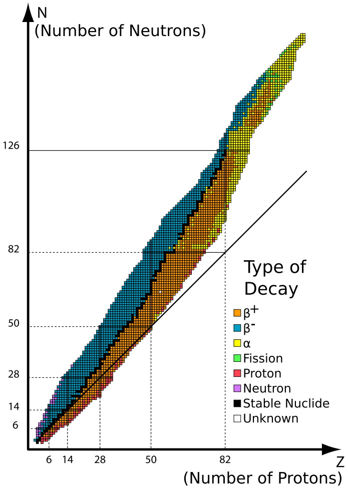
$$\begin{aligned}\Delta M_N &= M_n - M_p \\ &= 1.2933322(4)\,\mathrm{MeV} \\ &= 0.14\% \times M_N\end{aligned}$$

w/ $M_N = (M_n + M_p)/2$

Tiny but very important, e.g.

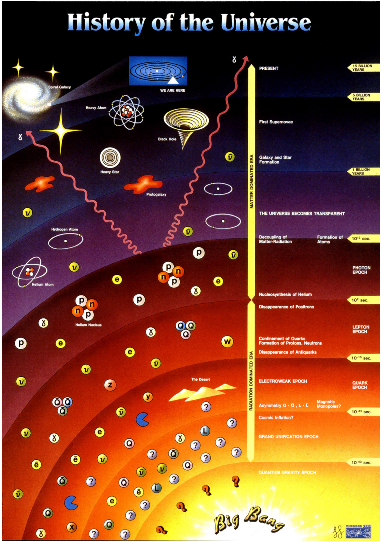
- required for stability of p and $^1\mathrm{H}$
- with $\Delta M_N < 0.05\% \times M_N$,
  $p + e^- \to n + \nu_e$
  $\to$ universe w/ mostly n
- determines valley of stability through β-decay

$\to$ necessary for stability of matter



Importance in the early universe

Time of interest here:
$1\ \mu\mathrm{s} \lesssim t \lesssim 3$ min



$$E_\beta = \Delta M_N - m_e - m_{\nu_e} = 0.08\% \times M_N$$

$$\downarrow$$

$$n \to p + e^- + \bar{\nu}_e \quad \text{in} \quad \tau_n \sim 15\ \text{min}$$

Critical for Big Bang nucleosynthesis (BBN)

If ΔM_N were larger and thus τ_n smaller

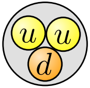
- $\to$ n decay before trapped and preserved in nuclei
- $\to$ easily get an universe without n !

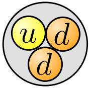
If $0.14\% > \Delta M_N/M_N \gtrsim 0.05\%$

- $\to$ much more ^4He and less p

$\to$ very finely tuned system
$\to$ goal: understand physics behind ΔM_N and similar phenomena

Why are *n* and *p* so similar?

proton: 

neutron: 

Very similar because differences between u and d very small on strong interaction scale
$\rightarrow$ nature has a near $SU(2)$ isospin symmetry

$$\begin{pmatrix} u \\ d \end{pmatrix} \longrightarrow \exp[i\vec{\theta}\cdot\frac{\vec{\tau}}{2}] \begin{pmatrix} u \\ d \end{pmatrix}$$

Only broken by small, often competing effects

	u	d
m_q [FLAG 13]	$2.16(11)\,\mathrm{MeV}$	$4.68(16)\,\mathrm{MeV}$
e_q	$\frac{2}{3}e$	$-\frac{1}{3}e$

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

Further importance of isospin breaking

- EM presently limiting factor in knowledge of m_u and m_d (e.g. FLAG 13)
  - $\rightarrow$ though very unlikely (e.g. FLAG 13), if $m_u = 0 \rightarrow$ solution to strong CP problem
  - $\rightarrow$ But: $m_u/M_p \sim 0.002$
- Important flavor observables are becoming very precisely known: e.g. $\mathrm{err}(m_{ud}), \mathrm{err}(m_s) \sim 2\%$, $\mathrm{err}(m_s/m_{ud}) \lesssim 1\%$, $\mathrm{err}(F_K) \sim 1\%$, $\mathrm{err}(F_K/F_\pi) \sim 0.5\%$, $\mathrm{err}(F_+^{K\pi}(0)) \sim 0.8\%$
  - $\rightarrow$ isospin breaking corrections required to improve indirect search for new physics

Can these effects be reliably computed in the fundamental theory?

Can be computed to low order in α & $(m_d - m_u) \ldots$

...but mixing w/ nonperturbative QCD

$\Rightarrow$ **nonperturbative QCD tool**
$\Rightarrow$ **include QED and $m_u \neq m_d$**

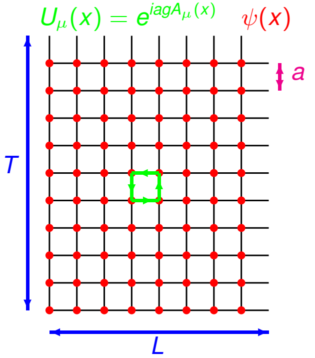
What is lattice QCD (LQCD)?

To describe ordinary matter, QCD requires $\geq$ 104 numbers at every point of spacetime
$\rightarrow \infty$ number of numbers in our continuous spacetime
$\rightarrow$ must temporarily "simplify" the theory to be able to calculate *(regularization)*
$\Rightarrow$ Lattice gauge theory $\longrightarrow$ mathematically sound definition of NP QCD:

- UV (& IR) cutoff $\rightarrow$ well defined path integral in Euclidean spacetime:

$$\begin{aligned}\langle O\rangle &= \int \mathcal{D}U\mathcal{D}\bar{\psi}\mathcal{D}\psi\, e^{-S_G-\int \bar{\psi}D[M]\psi}\, O[U,\psi,\bar{\psi}] \\ &= \int \mathcal{D}U\, e^{-S_G}\, \det(D[M])\, O[U]_{\text{Wick}}\end{aligned}$$

- $\mathcal{D}Ue^{-S_G}\det(D[M]) \geq 0$ & finite # of dofs $\rightarrow$ evaluate numerically using stochastic methods



LQCD is QCD when $m_q \rightarrow m_q^{\text{phys}}$, $a \rightarrow 0$ (after renormalization), $L \rightarrow \infty$ (and stats $\rightarrow \infty$)

HUGE conceptual and numerical ($\sim 10^9$ dofs) challenge

Huge progress in lattice QCD simulations

A little over 10 years ago we were stuck:

- Cost of calculations scaled very poorly as:
  - $m_{ud} \searrow m_{ud}^{\rm phys}$
  - $a \searrow 0$

  $\Rightarrow$ stuck with $m_{ud} \gtrsim 15 m_{ud}^{\rm phys}$ and $a \gtrsim 0.1\,\mathrm{fm}$

  $\Rightarrow$ too far away to make controlled contact with Nature

In past years, thanks to the work of many: (Sexton et al '92, Hasenbusch '01, Urbach et al '06, Lüscher '04, Del Debbio et al '06, Lüscher '07, BMWc '08, Blum et al '12, Frommer et al '13, . . .)

- Insights into how lattice QCD challenges our algorithms and better understanding of the dynamics of the Hybrid Monte Carlo

$\Rightarrow$ innovative solutions based on modern numerical mathematics

$\Rightarrow$ design of more effective discretizations of QCD

- Arrival of multi-Tflop/s $\rightarrow$ Pflop/s supercomputers
- Optimization of algorithms and codes for available resources

$\Rightarrow$ tools to perform % level QCD calculations . . . of “simple” quantities

$\Rightarrow$ need large number of simulations over large range of relevant parameters to control all systematics

Hadron spectrum and mass of ordinary matter

$\rightarrow$ validation of QCD as theory of strong interaction at low energy, in nonperturbative domain

$\rightarrow$ validation of mechanism that gives mass to ordinary matter

- $> 99\%$ of mass of visible universe is in the form of p & n
- $< 5\%$ of mass of p & n comes from mass of quark constituents
- Light hadron masses generated by QCD energy imparted to q and g via:

$$m = E/c^2$$

- mechanism at origin of $\gtrsim 95\%$ of mass of visible universe

- Higgs "only" gives masses to the q in N, whose sum $< 2\%$ of M_N

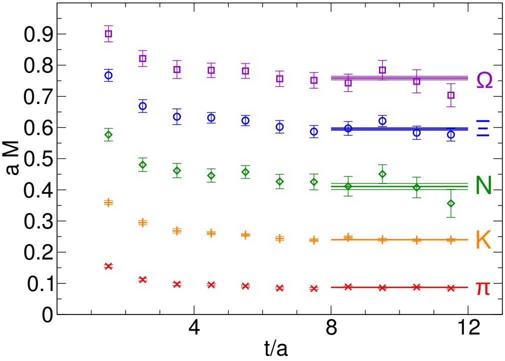
Hadron mass extraction

e.g. in pseudoscalar channel, M_π from correlated fit

$$C(t) \equiv \frac{1}{(L/a)^3} \sum_{\vec{x}} \langle [\bar{d}\gamma_5 u](x)[\bar{u}\gamma_5 d](0)\rangle \stackrel{0\ll t\ll T}{\longrightarrow} \frac{\langle 0|\bar{d}\gamma_5 u|\pi^+(\vec{0})\rangle\langle\pi^+(\vec{0})|\bar{u}\gamma_5 d|0\rangle}{2M_\pi} e^{-M_\pi t}$$

Can define an effective mass

$$aM(t+a/2) = \log[C(t)/C(t+a)] \stackrel{0\ll t\ll T}{\longrightarrow} aM_\pi$$



Effective masses for simulation at $a \approx 0.085\,\mathrm{fm}$ and $M_\pi \approx 0.19\,\mathrm{GeV}$

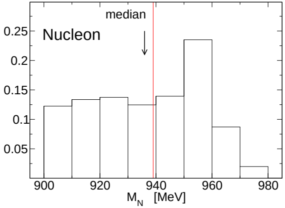
Ab initio calculation of light hadron masses

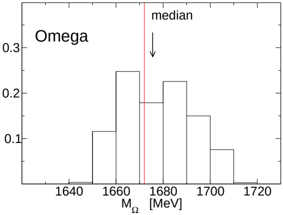
Dürr et al [BMWc], Science 322 (2008) 1224

BMWc '08 set: 20 large scale $N_f = 2 + 1$ simulations w/ $M_\pi \gtrsim 190\,\mathrm{MeV}$, $3a$'s $\approx 0.065 \div 0.125\,\mathrm{fm}$ and $L \nearrow 4\,\mathrm{fm}$

- Correct treatment of resonant states
- Perform 432 independent full analyses of our data for 12 particles . . .

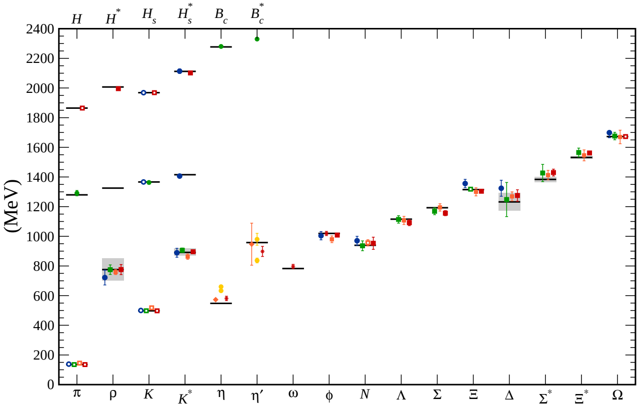
  $\Rightarrow$ systematic error distributions for the hadron masses by weighing each result w/ its fit quality





- Median $\rightarrow$ central value
- Central 68% CI $\rightarrow$ systematic error
- Repeat procedure for 2000 independent bootstrap samples
  $\rightarrow$ statistical error from central 68% CI of bootstrap distribution of medians

Lattice QCD and the hadron spectrum



- From Kronfeld '12
- Light hadrons: BMWc Science '08, MILC '04-'10, PACS-CS '09, QCDSF '11
- η, η': RBC/UKQCD '10, HadSpec '11, HPQCD '12
- ω: HadSpec '11
- Heavy-light (b-light shifted by $-4\,\mathrm{GeV}$): MILC '11, HPQCD '11, Mohler et al '11
- Also ETM '14, ...

$\rightarrow$ mass generation mechanism checked at few % level

$\rightarrow$ impressive validation of nonperturbative QCD

Including isospin breaking on the lattice

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

with $j_\mu = \bar{q}Q\gamma_\mu q$

(1) operator insertion method

$$\langle\mathcal{O}\rangle_{\text{QCD+QED}} = \langle\mathcal{O}\rangle^{\text{iso}}_{\text{QCD}} - \underbrace{\frac{1}{2}(m_u - m_d)\langle\mathcal{O}\int(\bar{u}u - \bar{d}d)\rangle^{\text{iso}}_{\text{QCD}}}_{(a)}$$

$$+\underbrace{\frac{1}{2}e^2\langle\mathcal{O}\int_{xy} j_\mu(x)D_{\mu\nu}(x-y)j_\nu(y)\rangle^{\text{iso}}_{\text{QCD}}}_{(b)} + \text{hot}$$

(2) direct method

Include $m_u \neq m_d$ and QED directly in simulation

Including isospin breaking on the lattice (cont'd)

What has been done:

- $m_u \neq m_d$ in valence only (MILC '09, Blum et al '10, Laiho et al '11, QCDSF/UKQCD '12, BMWc '10-, . . .)
  - ✓ no new simulations
  - ✓ error of $O(\alpha) \Rightarrow$ use phenomenology
- (a) (RM123 '12) and (b) (RM123 '13) of operator insertion method tried w/out quark-disconnected contributions
  - ✓ no new simulations
  - × error of $O(\alpha(m_s - m_{ud})/(N_c M_{\mathrm{QCD}}))$
- QED & $m_u \neq m_d$ in valence only (Eichten et al '97, Blum et al '07, '10, BMWc '10-, MILC '10-)
  - ✓ no new simulations
  - × error of $O(\alpha(m_s - m_{ud})/(N_c M_{\mathrm{QCD}}))$
- QED (Blum et al '12) & $m_u \neq m_d$ (PACS-CS '12) in sea w/ reweighting
  - ✓ as good as full simulation
  - × exponentially expensive in the volume
  - × only tried w/ low statistics in a single simulation $\rightarrow$ not very conclusive

QCD + QED à la BMWc

Dürr 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 $< 20\%$

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)
- 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)
- consistently renormalize QCD+QED theory
  $\rightarrow$ renormalize α using Wilson flow (Lüscher '10, 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)

Discretization of QED

To avoid phase transition issues, use non-compact formulation of QED (Duncan et al '96)

$\Rightarrow$ remains gauge invariant on lattice but must fix gauge

$\Rightarrow$ naively discretize Maxwell action in Feynman gauge:

$$S_\gamma[A_\mu(x)] = -\frac{a^4}{4}\sum_{\mu,\nu,x}(\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x))^2$$

w/ ∂_μ a finite difference operator

$\rightarrow$ transform to Coulomb gauge, $\vec{\nabla}\cdot\vec{A} = 0$, to have well defined Hamiltonian

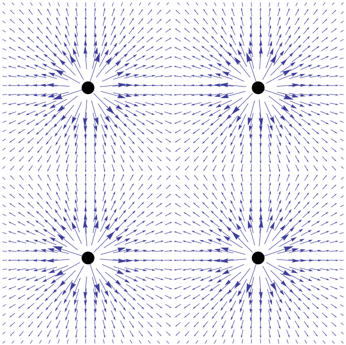
$\rightarrow$ couple photons to quarks through gauge-invariant lattice action

$$\sum_x \bar{\psi}(x)D[U]\psi(x) \qquad \text{w/} \qquad U_\mu = e^{iaeqA_\mu}U_\mu^{\mathrm{QCD}}$$

and qe the charge of the quark

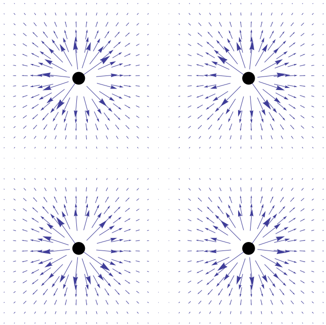
QED in finite volume

EM field of a point charge cannot be made periodic & continuous



$\longrightarrow$

Introduce small modification of QED e.o.m. $\sim 1/L^3$ which makes this possible



- Induces finite-volume effects $\sim \alpha/L$ that must be subtracted
  $\rightarrow$ small on QCD quantities but significant for isospin splittings

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

$$\underbrace{\alpha \int \frac{d^4k}{(2\pi)^4} \frac{1}{k^2} \cdots}_{\substack{\uparrow \\ \text{possible IR divergences} \\ \text{but not in physical qties}}} \quad \longrightarrow \quad \underbrace{\frac{\alpha}{TL^3} \sum_k \frac{1}{k^2} \cdots}_{\substack{\uparrow \\ \text{contains a straight 1/0!}}}$$

- HMC algorithm is ineffective in updating the zero mode

Finite-volume QED and zero-mode problem

Problem can be solved by **removing zero mode(s)**

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

$\rightarrow$ does not change infinite-volume physics

$\rightarrow$ physically equivalent to adding a canceling uniform charge distribution

- different schemes $\rightarrow$ different finite-volume behaviors
- some schemes more interesting than others

QED_{TL} zero-mode subtraction

- Set $\tilde{A}_\mu(k=0)=0$ on $T\times L^3$ four-torus (Duncan et al '96)
- Used in most previous studies
- Violates reflection positivity!

  $\rightarrow$ no Hamiltonian

  $\rightarrow$ divergences when L fixed, $T\rightarrow\infty$

$$\frac{\alpha}{TL^3}\sum_{k\neq 0}\frac{1}{k^2}\cdots \quad \xrightarrow[T\rightarrow+\infty, L\ \text{fixed}]{} \quad \alpha\int\frac{dk_0}{2\pi}\frac{1}{L^3}\sum_{\vec{k}}\frac{1}{k^2}\cdots$$

Checked analytically in 1-loop spinor (also scalar) QED calculation

$$m(T,L) \underset{T,L\rightarrow+\infty}{\sim} m\left\{1-q^2\alpha\left[\frac{\kappa}{2mL}\left(1+\frac{2}{mL}\left[1-\frac{\pi}{2\kappa}\frac{T}{L}\right]\right)\right.\right.$$
$$\left.\left.-\frac{3\pi}{(mL)^3}\left[1-\frac{\coth(mT)}{2}\right]-\frac{3\pi}{2(mL)^4}\frac{L}{T}\right]\right\}$$

up to exponential corrections, with $\kappa = 2.837\cdots$

QED$_L$ zero-mode subtraction

- 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 (orginally suggested in Hayakawa & Uno '08)
- Satisfies reflection positivity

  $\rightarrow$ fixing to Coulomb gauge, $\vec{\nabla}\cdot\vec{A}=0$, ensures existence of Hamiltonian

  $\rightarrow$ well defined asymptotic states

  $\rightarrow$ well defined $T, L\rightarrow\infty$ limit

Checked analytically in 1-loop spinor (and scalar) QED calculation

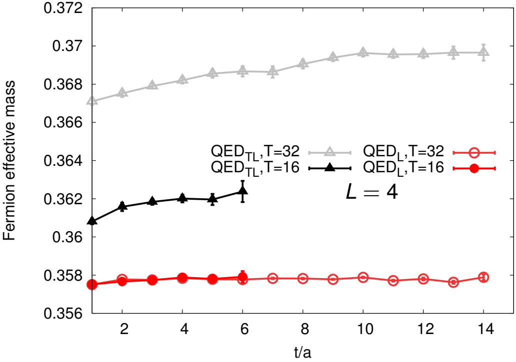
$$m(T,L) \underset{T,L\to+\infty}{\sim} m\left\{1-q^2\alpha\left[\frac{\kappa}{2mL}\left(1+\frac{2}{mL}\right)-\frac{3\pi}{(mL)^3}\right]\right\}$$

up to exponential corrections, with $\kappa=2.837\cdots$

$\Rightarrow$ only inverse powers of L and no powers in T

QED_{TL} vs QED_L: numerical tests

Numerical studies in pure spinor QED (w/out QCD)



QED_{TL}, as expected, has:

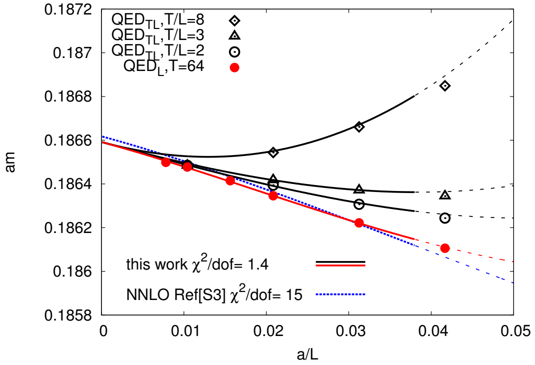
- no clear mass plateaux
- mass increases w/ T

As predicted, QED_L has none of these problems:

- ground state dominates at large t/a
- T-independent mass

QED_{TL} vs QED_L: numerical tests

Test pure QED simulations against our 1-loop finite-volume predictions



- Excellent agreement
- Both schemes give the same result in infinite volume
- QED_L cleaner and has more controlled infinite-volume limit

QED_L finite-volume effects for composite particles

How about QED_L FV effects on composite particles (e.g. hadrons)?

In our point spinor and scalar QED_L calculations find

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

independent of particle spin

Same result found for:

- Mesons in $SU(3)$ PQ χPT (Hayakawa et al '08)
- Mesons/baryons in non-relativistic EFT (Davoudi et al '14)

$\rightarrow$ leading $1/L$ and $1/L^2$ terms independent of particle spin and structure?

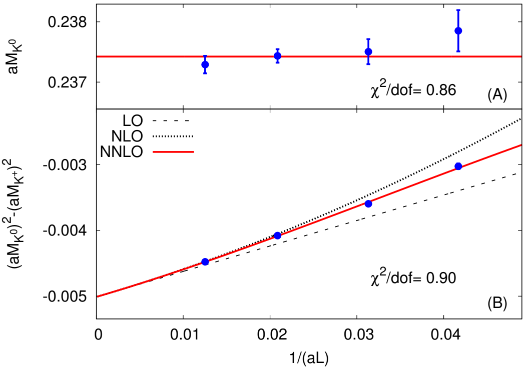
For a general field theory, this universality **follows from Ward identities** (BMWc '14), assuming:

- the photon is the only massless asymptotic state
- the charged particle considered is stable and non-degenerate in mass

$\rightarrow$ leading FV effects can be removed analytically

FV effects in kaon masses

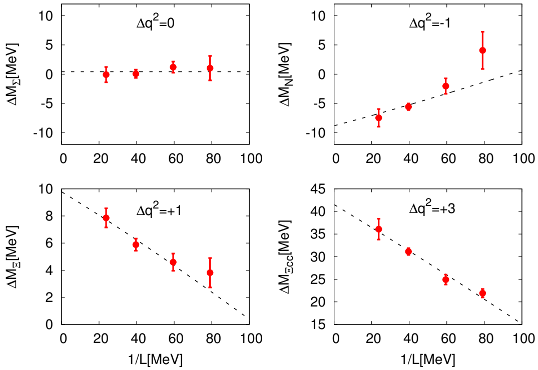
Dedicated FV study w/ $L = 2.4 \nearrow 8.0\,\mathrm{fm}$ and other parameters fixed (bare $\alpha \sim 1/10$, $M_\pi = 290\,\mathrm{MeV}$, $M_{K^0} = 450\,\mathrm{MeV}$, $a = 0.10\,\mathrm{fm}$)



- 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

FV effects in baryon masses

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



- $\Delta M_\Sigma = M_{\Sigma^+} - M_{\Sigma^-}$ shows no volume dependence ($\Delta q^2 = 0$)
- Strategy: fix universal $1/L$, $1/L^2$ terms and add $1/L^3$ if required

Dynamical QED and autocorrelations

Long range QED $\rightarrow$ huge autocorrelations in standard HMC, even in free case (uncoupled oscillators)

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

$$\rightarrow A_{\mu,k}(\tau) = A_{\mu,k}(0) \cos(|\hat{k}|\tau) + \frac{\Pi_{\mu,k}}{|\hat{k}|} \sin(|\hat{k}|\tau)$$

and small k modes practically unchanged after $\tau = 1$ trajectory

Solution: give system k-dependent mass M_k

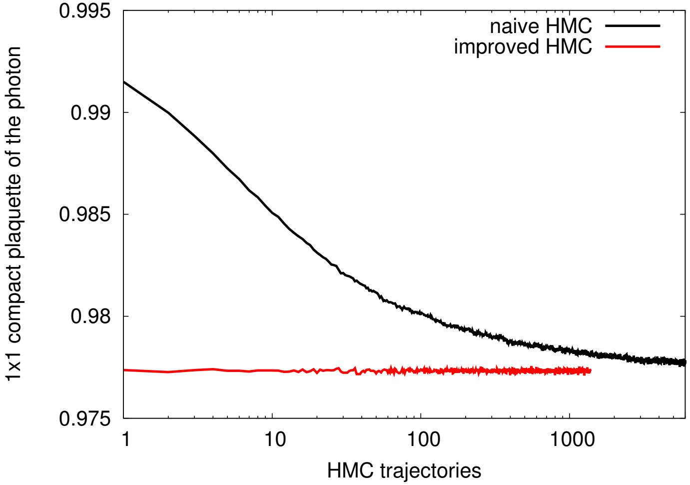
$$\mathcal{H} = \frac{1}{2V} \sum_{\mu,k} \left\{ \frac{|\Pi_{\mu,k}|^2}{M_k} + \hat{k}^2 |A_{\mu,k}|^2 \right\} \quad \text{with} \quad M_k = \frac{4\hat{k}^2}{\pi^2}$$

$$\rightarrow A_{\mu,k}(\tau) = A_{\mu,k}(0) \cos(\frac{\pi}{2}\tau) + \frac{\pi}{2} \frac{\Pi_{\mu,k}}{\hat{k}^2} \sin(\frac{\pi}{2}\tau)$$

and all memory of initial condition forgotten at $\tau = 1$ for all k

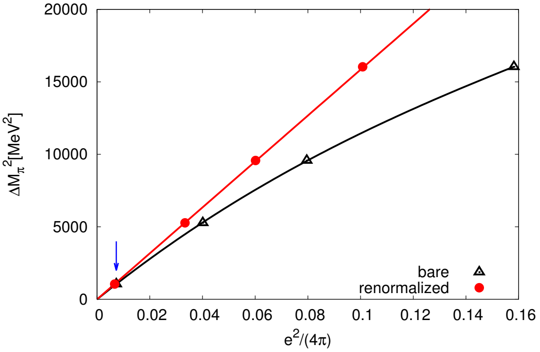
$\rightarrow$ only works w/ zero-mode subtraction

Dynamical QED and autocorrelations



Requires an FFT in every HMC step

Renormalization of α



- $\Delta M_\pi^2 = M_{\pi^+}^2 - M_{“\pi^0”}^2$ is not linear in $\alpha_{\rm bare}$
- Becomes so in terms of $\alpha_{\rm ren}$ renormalized around scale of processes involved

$\Rightarrow$ simulate for 5 values $\alpha_{\rm bare} \in [0, 0.16]$

$\Rightarrow$ interpolate linearly in $\alpha_{\rm bare}$ to physical value

Renormalization of α

- Use Wilson flow (Lüscher '10) (discretized version of):

$$\frac{\partial B_\mu(\tau;x)}{\partial\tau} = -\partial_\nu F^{(B)}_{\mu\nu}(\tau;x), \qquad E(\tau) = \tau^2 \int_x F^{(B)}_{\mu\nu}(\tau;x) F^{(B)}_{\mu\nu}(\tau;x)$$

  with $B_\mu(\tau=0;x) = A_\mu(x)$

- Then define

$$\alpha_{\rm ren}(\tau) = Z(\tau)\alpha_{\rm bare} \qquad \text{w/} \qquad Z(\tau) = \langle E(\tau)\rangle / E_{\rm tree}(\tau)$$

- Sizeable FV effects can be corrected by considering $E_{\rm tree}(\tau)$ in FV

- Choose renormalization scale $(8\tau)^{1/2} \simeq 280 \nearrow 525\,\mathrm{MeV}$ and match $\alpha_{\rm ren}(\tau)$ to Thomson limit

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

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

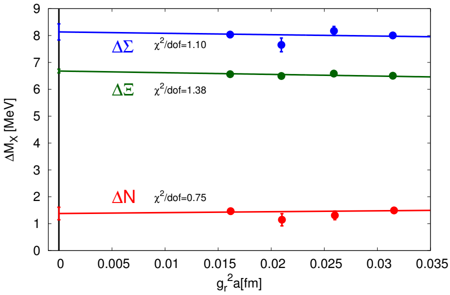
  - Weight different analyses w/

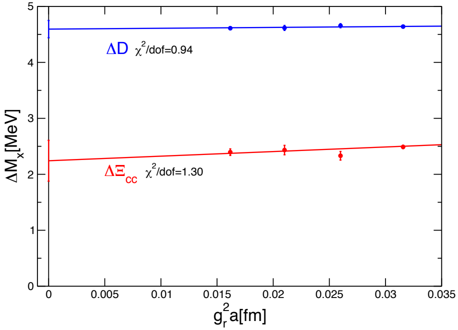
$$\exp\left[-(\mathrm{AIC} - \mathrm{AIC}_{\rm min})/2\right]$$

  - 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

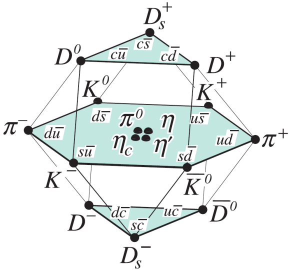
Continuum extrapolations

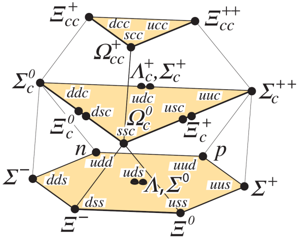


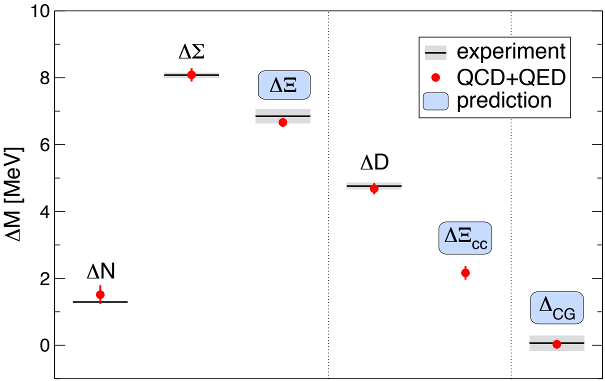


Continuum extrapolations smooth even in presence of valence (and sea) charm

Results for isospin mass splittings







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

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

- At LO in α and $\delta m \equiv (m_d - m_u)$ can separate

$$\Delta M_X = \Delta_{\rm QED} M_X + \Delta_{\rm QCD} M_X$$

w/ first term $\propto \alpha$ and second $\propto \delta m$

- Intrinsic scheme ambiguity of $O(\alpha\delta m, \alpha^2, \delta m^2, \alpha m_{ud})$

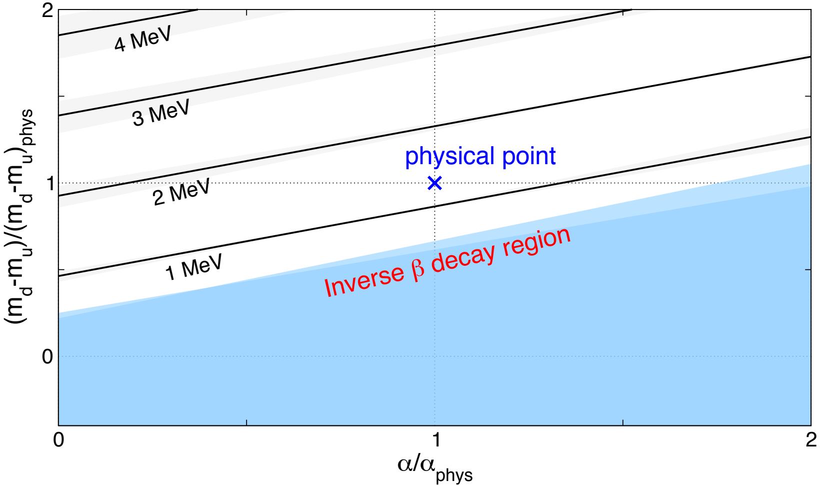
- ΔM_Σ largely dominated by δm contribution

$\rightarrow$ use $\Delta_{\rm QED} M_\Sigma \equiv 0$ to define separation
$\rightarrow$ sufficient for current level of precision

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

Nature's fine tuning

Use PDG '14 ΔM_N to get $\Delta_{\text{QCD}} M_N / \Delta_{\text{QED}} M_N = -2.49(23)(29)$ and



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