Ab-initio calculation: neutron-proton mass difference

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why do we have mass at all?
could the world look different?

Lattice QCD talk

Outline

1. Introduction
2. Action
3. Finite V
4. QED coupling
5. Results
6. Summary

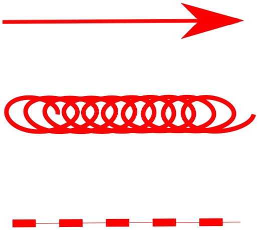
Ordinary matter: three types of particles $\Rightarrow$ H, He ...

ELECTRON	U-QUARK	D-QUARK
e	u	d

ELECTRIC

STRONG

HIGGS



All of them are massless!

ELECTRON U-QUARK D-QUARK

e u d

$m_e=0$ $m_u=0$ $m_d=0$

Why do we have mass at all?

Why do not we just fly apart with c?

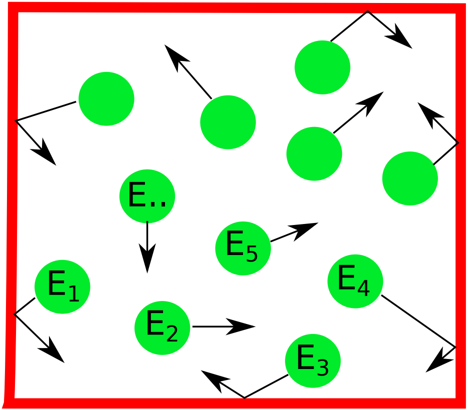
Three mechanisms

I. Strong mass

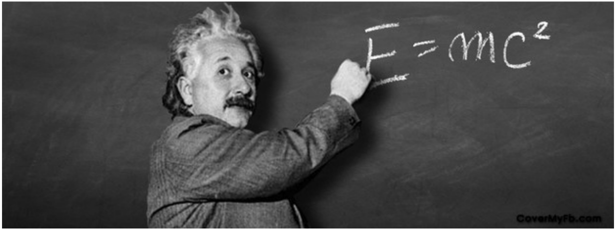
II. Electromagnetic mass

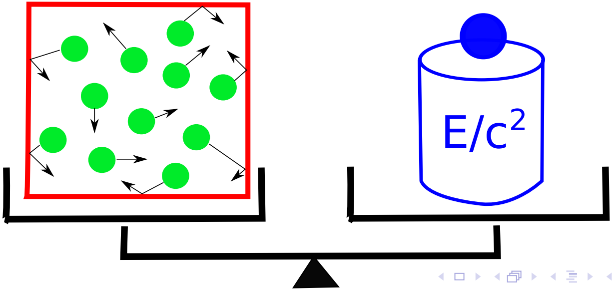
III. Mass from the Higgs-Mechanism

The massless box

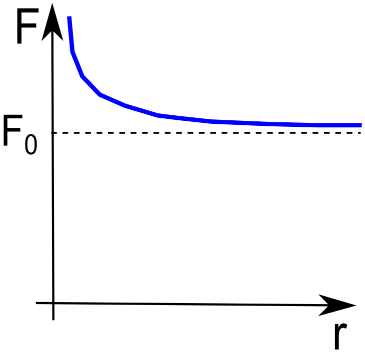


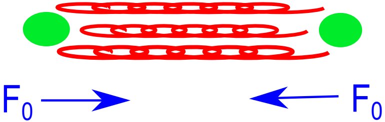
Mass from energy





The strong force (massless box) $\Longrightarrow$ hadrons





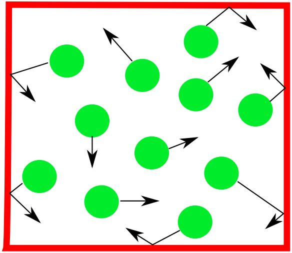
Quarks can not fly apart

they are confined!

Three mechanisms

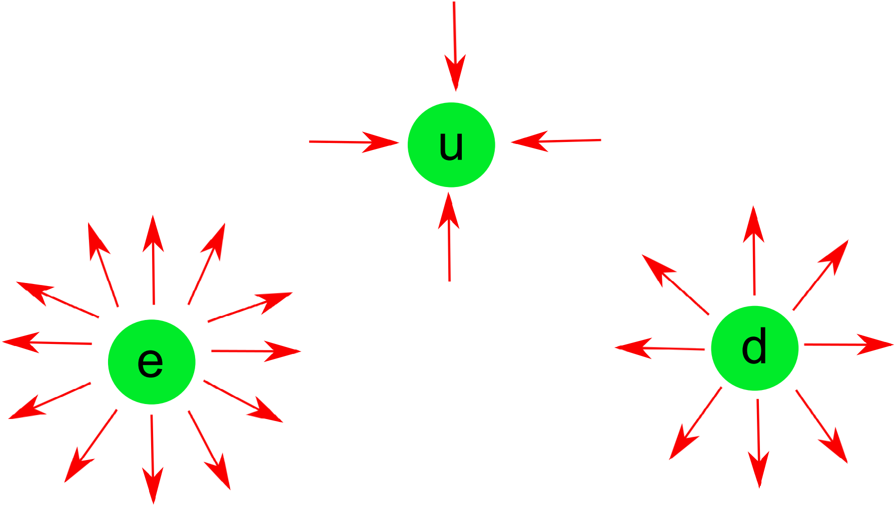
STRONG

ELECTRIC

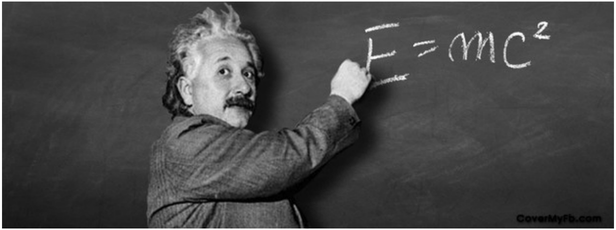


HIGGS

The electric field



Electric energy from the field energy



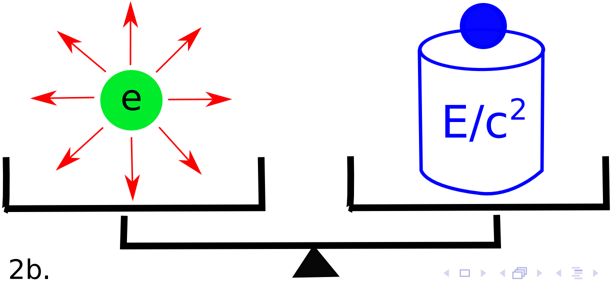
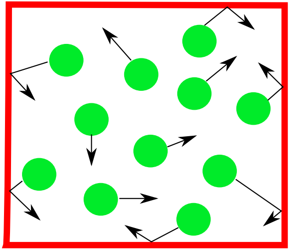


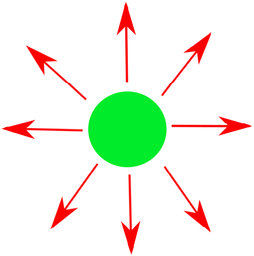
FIG. 2b.

Three mechanisms

STRONG

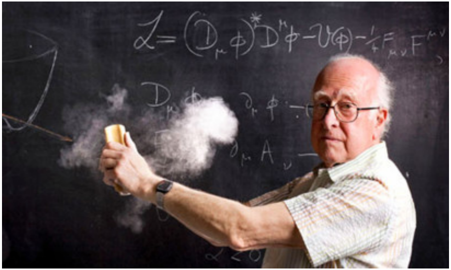


ELECTRIC

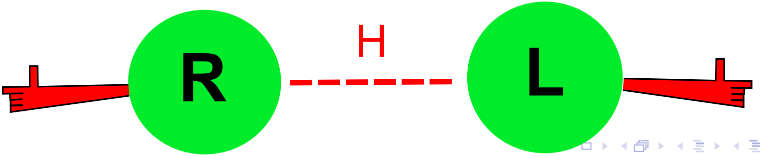


HIGGS

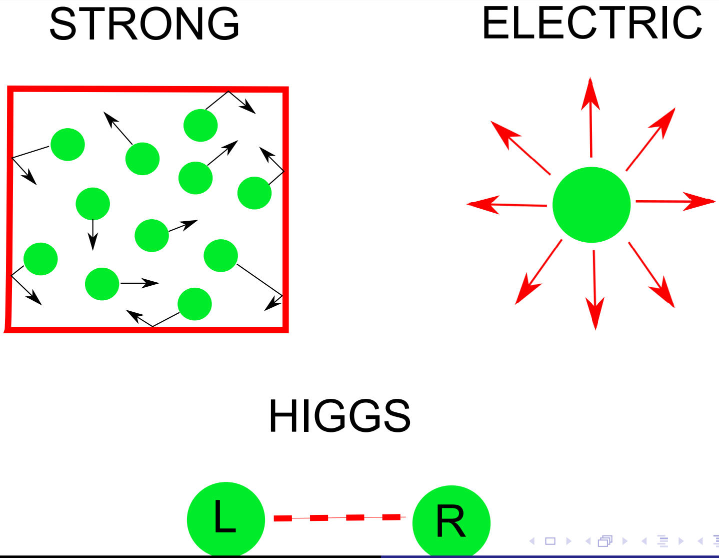
Higgs-Mechanism: Yukawa couplings



MASSLESS $\longrightarrow$ **MASSIVE**

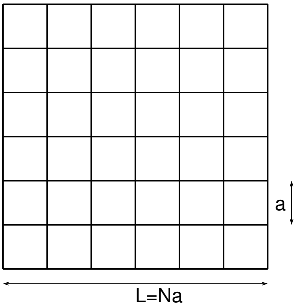


Three mechanisms



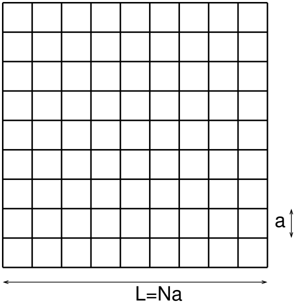
Continuum limit

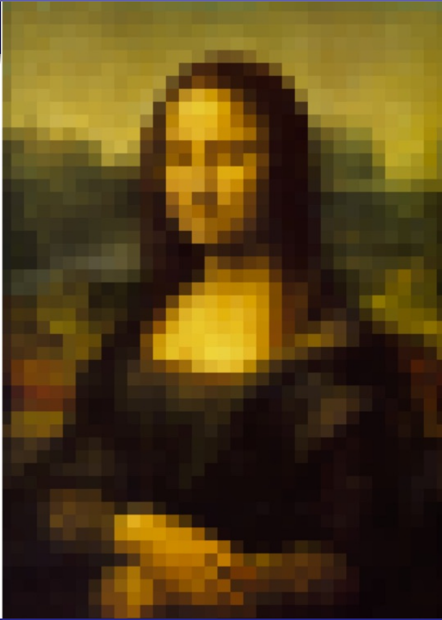
- lattice action: discretize the Lagrangian of QCD on a space-time grid



Continuum limit

- lattice action: discretize the Lagrangian of QCD on a space-time grid
- repeat the calculation on finer and even finer lattices





Continuum limit

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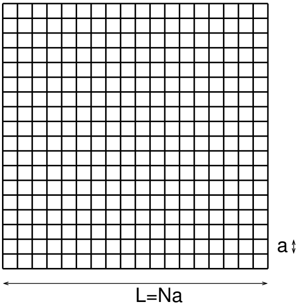
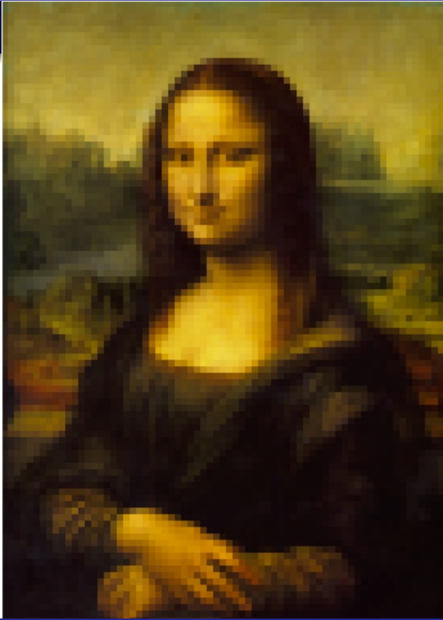
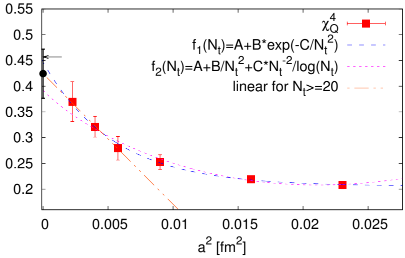




Continuum limit

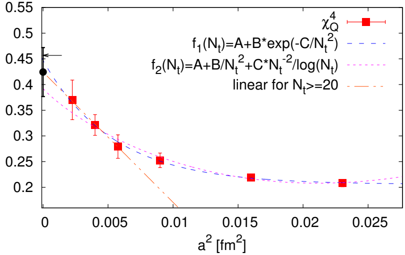
- lattice action: discretize the Lagrangian of QCD on a space-time grid
- repeat the calculation on finer and even finer lattices

$\Rightarrow$ continuum limit extrapolation



Continuum limit

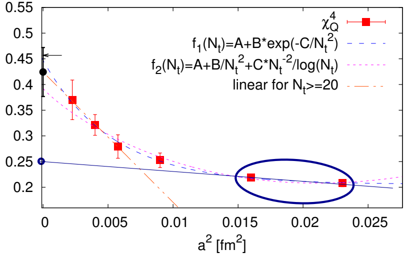
- observables are affected by discretization effects quite differently



Continuum limit

- observables are affected by discretization effects quite differently

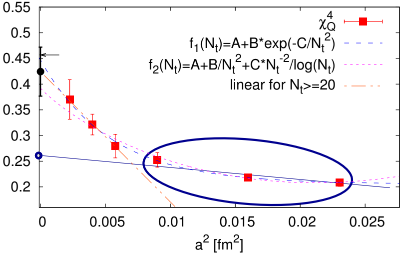
- in quantitative predictions cut-off efects can be misleading



Continuum limit

• observables are affected by discretization effects quite differently

• in quantitative predictions cut-off efects can be misleading
$\Rightarrow$ or even completely wrong



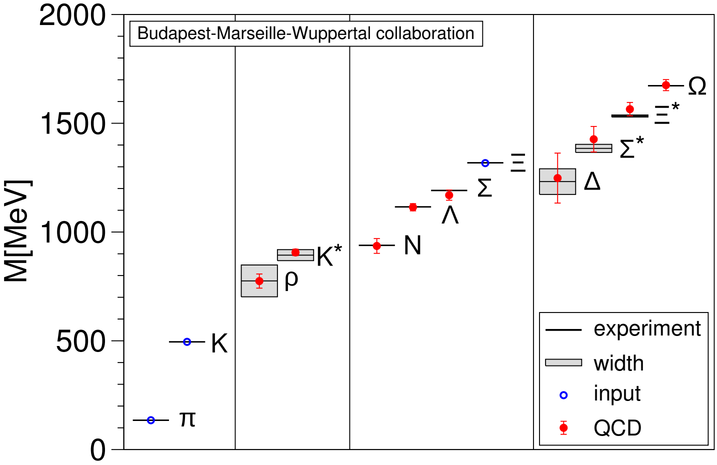
FLAG review of lattice results

Colangelo et al. Eur.Phys.J. C71 (2011) 1695

Collaboration	publication status	chiral extrapolation	continuum extrapolation	finite volume	renormalization	running	$m_{ud,\overline{\mathrm{MS}}(2\mathrm{GeV})}$	$m_{s,\overline{\mathrm{MS}}(2\mathrm{GeV})}$
PACS-CS 10	P	★	■	■	★	*a*	2.78(27)	86.7(2.3)
MILC 10A	C	●	★	★	●	–	3.19(4)(5)(16)	–
HPQCD 10	A	●	★	★	★	–	3.39(6)*	92.2(1.3)
BMW 10AB	P	★	★	★	★	*b*	3.469(47)(48)	95.5(1.1)(1.5)
RBC/UKQCD	P	●	●	★	★	*c*	3.59(13)(14)(8)	96.2(1.6)(0.2)(2.1)
Blum et al. 10	P	●	■	●	★	–	3.44(12)(22)	97.6(2.9)(5.5)

Final result for the hadron spectrum

S. Durr et al., Science 322 1224 2008



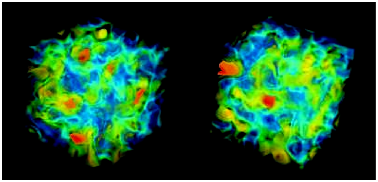
Breakthrough of the Year

Proton's Mass 'Predicted'

STARTING FROM A THEORETICAL DESCRIPTION OF ITS INNARDS, physicists precisely calculated the mass of the proton and other particles made of quarks and gluons. The numbers aren't new; experimenters have been able to weigh the proton for nearly a century. But the new results show that physicists can at last make accurate calculations of the ultracomplex strong force that binds quarks.

In simplest terms, the proton comprises three quarks with gluons zipping between them to convey the strong force. Thanks to the uncertainties of quantum mechanics, however, myriad gluons and quark-antiquark pairs flit into and out of existence within a proton in a frenzy that's nearly impossible to analyze but that produces 95% of the particle's mass.

To simplify matters, theorists from France, Germany, and Hungary took an approach known as "lattice quantum chromodynamics."



They modeled continuous space and time as a four-dimensional array of points—the lattice—and confined the quarks to the points and the gluons to the links between them. Using supercomputers, they reckoned the masses of the proton and other particles to a precision of about 2%—a tenth of the uncertainties a decade ago—as they reported in November.

In 2003, others reported equally precise calculations of more-esoteric quantities. But by calculating the familiar proton mass, the new work signals more broadly that physicists finally have a handle on the strong force.

Introduction to isospin symmetry

Isospin symmetry: 2+1 or 2+1+1 flavor frameworks

if 'up' and 'down' quarks had identical properties (mass,charge)

$M_n = M_p, \quad M_{\Sigma^+} = M_{\Sigma^0} = M_{\Sigma^-}, \quad$ etc.

The symmetry is explicitly broken by

- up, down quark electric charge difference (up: 2/3·e down:-1/3·e)

$\Rightarrow$ proton: uud=2/3+2/3-1/3=1 whereas neutron: udd=2/3-1/3-1/3=0

at this level (electric charge) the proton would be the heavier one

- up, down quark mass difference ($m_d/m_u \approx 2$): 1+1+1+1 flavor

The breaking is large on the quark's level ($m_d/m_u \approx 2$ or charges) but small (typically sub-percent) compared to hadronic scales.

These two competing effects provide the tiny M_n-M_p mass difference $\approx$ 0.14% is required to explain the universe as we observe it

Big bang nucleosynthesys and nuclei chart

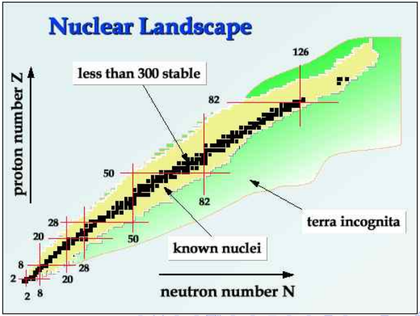
if $\Delta m_N < 0.05\%$ $\rightarrow$ inverse β decay leaving (predominantly) neutrons $\Delta m_N \gtrsim 0.05\%$ would already lead to much more *He* and much less *H* $\rightarrow$ stars would not have ignited as they did

if $\Delta m_N > 0.14\%$ $\rightarrow$ much faster beta decay, less neutrons after BBN burinng of *H* in stars and synthesis of heavy elements difficult

The whole nuclei chart is based on precise value of Δm_N

Could things have been different?

Jaffe, Jenkins, Kimchi, PRD 79 065014 (2009)



extension steps for a fully realistic theory

1. include dynamical charm:
usually easy since existing codes can include many fermions
since m_c is quite heavy it is computationally cheap
one needs small lattice spacings to have am_c small enough

2. include $m_u \neq m_d$ (similarly large effect as QED):
usually easy since existing codes can include many fermions
$m_u \approx m_d/2$: more CPU-demanding than 2+1 flavors
since m_u is small larger V needed to stabilize the algorithm:
more CPU but large V (upto 8 fm) is good for other purposes

3. include QED:
difficult, since the action/algorithmic setup must be changed
conceptual difficulties for finite V, since QED is not screened
additional computational costs are almost negligable

Lattice action

$$S[U, A, \overline{\psi}, \psi] = S_g[U; g] + S_\gamma[A] + \sum_f \overline{\psi}_f D[U, A; e, q_f, m_f]\psi_f.$$

QCD gauge action (S_g): tree level Symanzik action

Photon action (S_γ): non-compact formulation $\rightarrow$ action quadratic
gauge fixing is needed to determine charged particle propagators

$$S_\gamma[A] = \frac{1}{2TL^3} \sum_{\mu,k} |\hat{k}|^2 |A_{\mu,k}|^2$$

Dirac operator: tree level clover improved Wilson action
3 levels of HEX smearing for gluons
(photons included in exponential form after one smearing step)

Zero mode subtraction

The absence of a mass gap may cause divergences at finite volume
perturbative momentum sums $\rightarrow 1/k^2$ factors $\rightarrow$
zero mode problematic

Removing a finite number of modes does not change $V \rightarrow \infty$ physics

Advantages of zero mode removal:
$\rightarrow$ analytic calculation of finite V corrections is possible
$\rightarrow$ algorithmic speedup

Many possibilities, we study two choices:
QED_{TL}, global zero mode removal: $\sum_x A_{\mu,x} = 0 \quad \forall\mu$
QED_L (Hayakawa, Uno), all spatial zero modes: $\sum_{\vec{x}} A_{\mu,x_0,\vec{x}} = 0 \quad \forall\mu, x_0$

Most previous studies used QCD_{TL}

QED in a finite volume

Calculate 1 loop self energy of charged particles in finite and infinite volumes

For a point-like particle

$$\Delta\Sigma(p,T,L) = \left[\sum_k - \int \frac{d^4k}{(2\pi)^4}\right] \sigma(k,p)$$

the difference between the QED_{TL} and QED_L schemes is in the photon momentum sum:

QED_{TL}: $\sum_k \equiv \frac{1}{TL^3} \sum_{k\neq 0}$
QED_L: $\sum_k \equiv \frac{1}{TL^3} \sum_{k_0} \sum_{\vec{k}\neq 0}$

Finite V correction to the pole mass can be calculated

$\Delta\Sigma$ both UV and IR finite, no further regularization needed.

Result for a spin half particle in QED_{TL}:

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

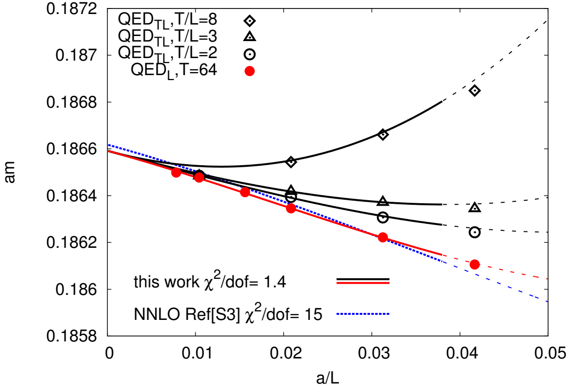
with $\kappa = 2.837297(1)$

Diverges for $T/L \to \infty$!

In QED_L the correction is T independent:

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

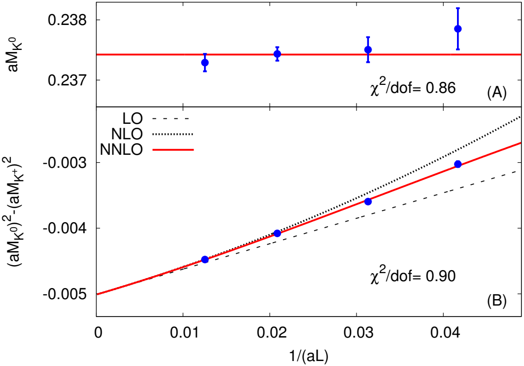
L dependence in the two schemes



The two schemes give the same result as long as $L \to \infty$ at fixed T

QED_L does not diverge for small L-s

Finite V dependence of the kaon mass



Neutral kaon shows essentially no (small $1/L^3$) volume dependence
Volume dependence of the K splitting is perfectly described
$1/L^3$ order is significant for kaon (baryons are not as precise)

Lattice spacings and pion masses

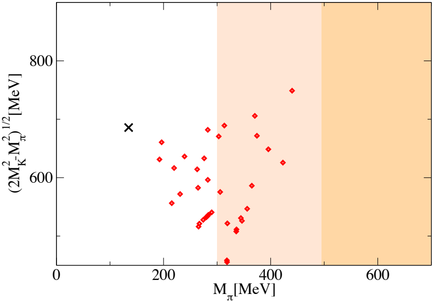
final result is quite independent of the lattice spacing & pion mass

$\Longrightarrow$ four lattice spacings with a=0.102, 0.089, 0.077 and 0.064 fm

four volumes for a large volume scan: L=2.4 ... 8.2 fm

five charges for large electric charge scan: e=0 ... 1.41

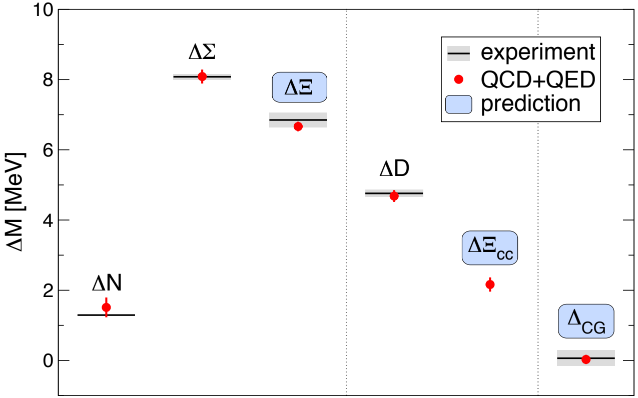
41 ensembles with M_π=195–440 MeV (various cuts)



large parameter space: helps in the Kolmogorov-Smirnov analysis

Isospin splittings

splittings in channels that are stable under QCD and QED:



ΔM_N, ΔM_Σ and ΔM_D splittings: post-dictions

ΔM_Ξ, $\Delta M_{\Xi_{cc}}$ splittings and $\Delta_{\rm CG}$: predicitions

Isospin splittings: numerical values

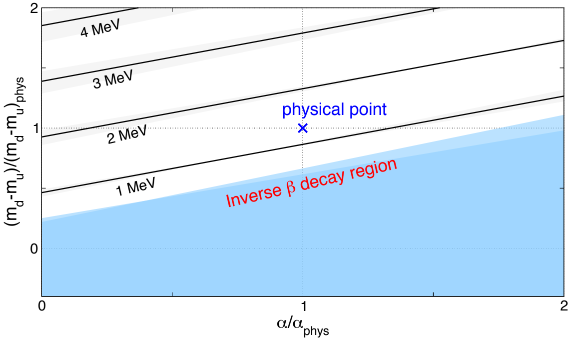
here we list also the individual contributions from QCD and QED

	splitting [MeV]	QCD [MeV]	QED [MeV]
ΔN=n-p	1.51(16)(23)	2.52(17)(24)	-1.00(07)(14)
$\Delta\Sigma=\Sigma^{-}$-Σ^{+}	8.09(16)(11)	8.09(16)(11)	0
$\Delta\Xi=\Xi^{-}$-Ξ^{0}	6.66(11)(09)	5.53(17)(17)	1.14(16)(09)
ΔD=$D^{\pm}$-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)
$\Delta_{\mathrm{CG}}=\Delta$N-$\Delta\Sigma+\Delta\Xi$	0.00(11)(06)	-0.00(13)(05)	0.00(06)(02)

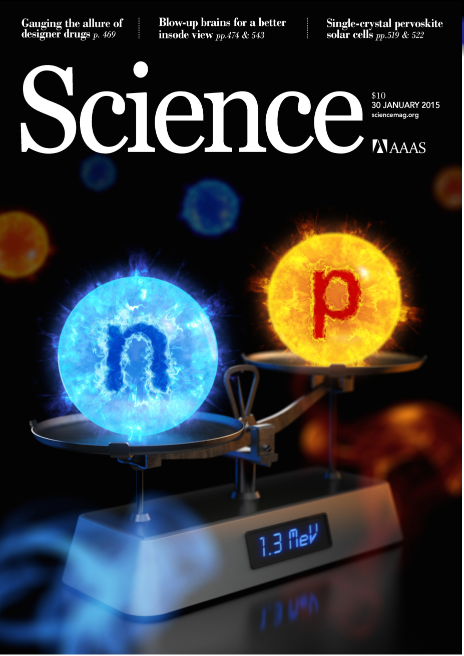
Quantitative anthropics

Precise scientific version of the great question:
Could things have been different (string landscape)?

eg. big bang nucleosynthesis & today's stars need $\Delta M_N \approx$ 1.3 MeV



(lattice message: too large or small α would shift the mass)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n
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1.3 MeV


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The mass difference between protons and neutrons
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Gang of three
How dynactin, dynein, and Bicaudal-D2 motor together
p. 1441

Summary

Motivations:

- neutrons are more massive than protons ΔM_N=1.3 MeV
- existence/stability of atoms (as we know them) relies on this fact
- splitting: significant astrophysical and cosmological implications
- genuine cancellation between QCD and QED effects: new level

Computational setup:

- 1+1+1+1 flavor full dynamical QCD+QED simulations
- four lattice spacings in the range of 0.064 to 0.10 fm
- pion masses down to 195 MeV
- lattice volumes up to 8.2 fm (large finite L corrections)

Technical novelties (missing any of them would kill the result):

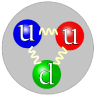
- dynamical QED_L: zero modes are removed on each time slice
- analytic control over finite L effects (larger than the effect)
- high precision numerics for finite L corrections
- large autocorrelation for photon fileds $\Rightarrow$ new algorithm
- improved Wilson flow for electromagnetic renormalization
- Kolmogorov-Smirnov analysis for correlators
- Akaike information criterion for extrapolation/interpolation
- fully blind analysis to extract the final results

$\Rightarrow$ all extrapolated to the continuum and physical mass limits

Results:

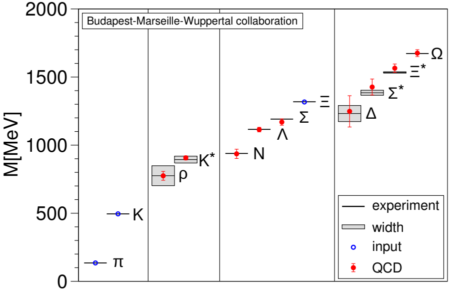
- ΔM_N is greater than zero by five standard deviations
- ΔM_N, ΔM_Σ and ΔM_D splittings: post-dictions
- ΔM_Ξ, $\Delta M_{\Xi_{cc}}$ splittings and $\Delta_{\rm CG}$: predicitions
- quantitative anthropics possible (fairly large region is OK)

The proton

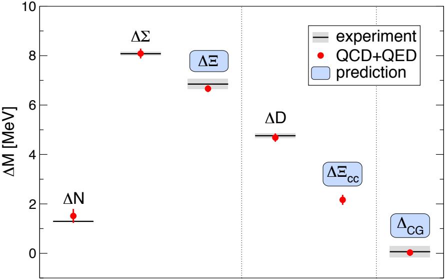


Strong + Higgs + Electro = Experiment

2008



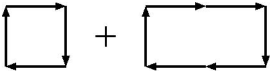
2014



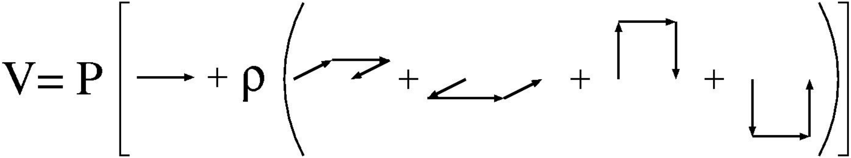
vision about a future, in which high precisions can be achieved
for a broad spectrum of non-perturbative questions (lattice formalism)

Choice of the action

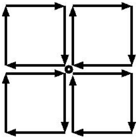
no consensus: which action offers the most cost effective approach
our choice: tree-level $O(a^2)$-improved Symanzik gauge action



6-level (stout) or 2/3-level (HEX) smeared improved Wilson fermions



with tree-level $O(a)$ clover improved fermions:



Further advantages of the action

stout smearing $\Rightarrow$ smallest eigenvalue of M: small fluctuations

C. Morningstar, M. J. Peardon, Phys. Rev. D69 054501, (2004)

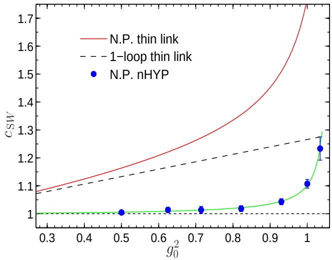
$\Rightarrow$ simulations are stable (major issue of Wilson fermions & speedup)

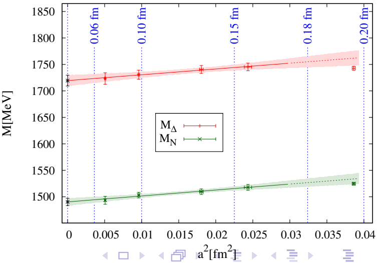
non-perturbative (improvement) coefficient: $\approx$ tree-level (smearing)

R. Hoffmann et al., PoS **LAT2007** (2007) 1 04

good a^2 scaling of hadron masses (M_π/M_ρ=2/3) up to $a\approx$0.2 fm

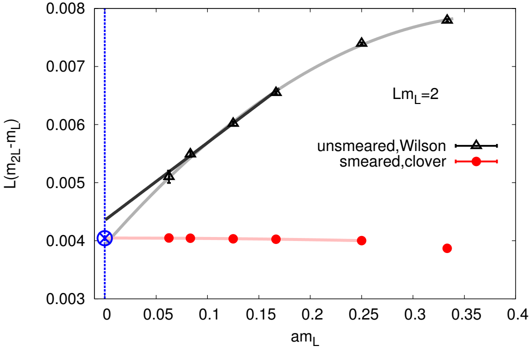
S. Dürr et al. [Budapest-Marseille-Wuppertal Collaboration] Phys. Rev. D79, 014501 (2009)





Continuum scaling of the QED action

Using a fixed physical volume (L) set the scale by finite V mass (m_L) and determine a finite volume effect $m_{2L} - m_L$
Comparison with 1 loop analytic results:



smearing and clover term dramatically improves scaling

Updating the photon field

Long range QED interaction $\rightarrow$ huge autocorrelation in standard HMC

Solution: HMC Hamiltonian in momentum space:

$$\mathcal{H} = \frac{1}{2TL^3} \sum_{\mu,k} \left\{ |\hat{k}|^2 |A_{\mu,k}|^2 + \frac{|\Pi_{\mu,k}|^2}{m_k} \right\}$$

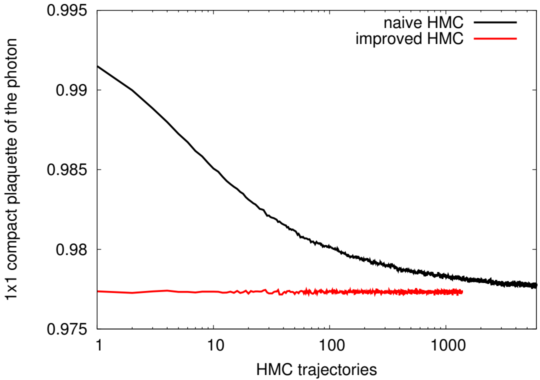
Use different masses for every mode:

$$m_k = 4|\hat{k}|^2/\pi^2$$

Every oscillator forgets initial condition at $t = 1 \rightarrow$ no autocorrelation
Only works with zero mode subtraction (due to $1/k^2$)
Zero mode subtraction is trivial

Coupling to quarks is in coordinate space $\rightarrow$ FFT in every step

Autocorrelation of the photon field



Standard HMC has $\mathcal{O}(1000)$ autocorrelation

Improved HMC has none (for the pure photon theory)

Small coupling to quarks introduces a small autocorrelation

Take couplings larger than 1/137

simulate at couplings that are larger than the physical one:
in such a case the signal outweighs the noise
precise mass and mass difference determination is possible

for e=0 and $m_u = m_d$ we know the isospin splittings exactly
$\Longrightarrow$ they vanish, because isospin symmetry is restored
$\alpha = e^2/4\pi \gg 1/137$ and e=0 can be used for interpolation

this setup will be enough to determine the isospin splittings
leading order finite volume corrections: proportional to α
leading order QED mass-splittings: proportional to α
no harm in increasing α, only gain (renormalization)

(perturbative Landau-pole is still at a much higher scale:
hundred-million times higher scale than our cutoff/hadron mass)

Choice of the physical QED coupling

eventually we want a. $\alpha = 1/137.036...$ b. in the Thomson limit
thus renormalizing it at the scale of the electron mass
our lattices are small to make measurements in this limit (0.5 MeV)

$\Rightarrow$ define the renormalized coupling at a hadronic scale
(we use the Wilson-flow to define the renormalization procedure)
the difference between the two is of order $O(\alpha^2)$
physical case (that is where we interpolate): relative difference 1%
can be neglected (perturbatively included): subdominant error

much more serious issue: L dependence of e_R (up to 20%)
can be removed by tree-level improvement of the flow

Tree-level improvement of the Wilson-flow

Wilson-flow for QED is a soluble case M. Luscher, 1009.5877

in the $t \to \infty$ case $t^2 \langle G_{\mu\nu} G_{\mu\nu} \rangle = 3e_R^2/32\pi^2$
which gives for our bare couplings renormalized ones: $Z = e_R^2/e^2$

on a finite lattice the flow is not yet $3e_R^2/32\pi^2$
it is proportional to the finite lattice sum:

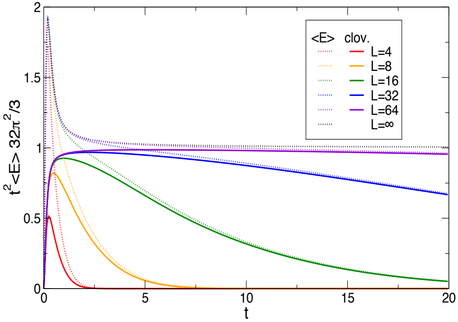
$$\frac{\tau^2}{TL^3} \sum_k \frac{\exp(-2|\hat{k}|^2\tau)}{|\hat{k}|^2} \left[\sum_{\mu \neq \nu} (1 + \cos k_\nu) \sin^2 k_\mu \right]$$

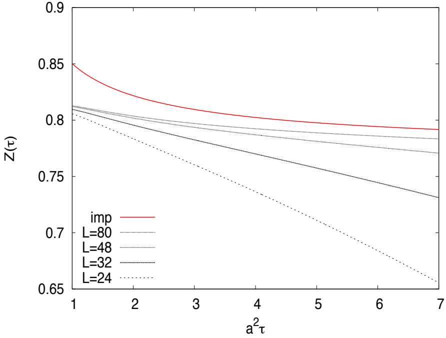
which indeed approaches $3/32\pi^2$ for $T, L, \tau \to \infty$

in our simulations: Z (relating e_R and e) must include this effect

Tree-level improved Z factors

$\Downarrow$ how in this limit (T,L,$\tau \to \infty$) can we reach $3/32\pi^2$





M_π=290 MeV & L=2.4–L=8.2 fm: Z with/without finite V correction $\Uparrow$

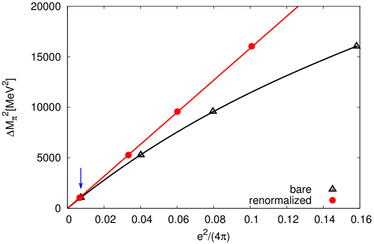
at small τ (cutoff scale) no sensitivity to the volume

for large τ sensitivity increases (up to 20%)

include factors between the finite/∞ V cases: curves coincide

Interpolation to the physical QED coupling

expansions in renormalized quantities behave usually better
(faster convergence than if one used bare quantities)
illustration (precise data): $\Delta M_\pi^2 = M_{du}^2 - (M_{\bar{u}u}^2 + M_{\bar{d}d}^2)/2$
(connected diagrams: ChPT tells us that it is purely electromagnetic)



large higher order terms if one uses the bare e
the splitting is linear in e_R (higher order terms are small)
true for all isosplin splitting channels (others: less sensitive)

The challenge of computing $M_n - M_p$ (on the 5σ level)

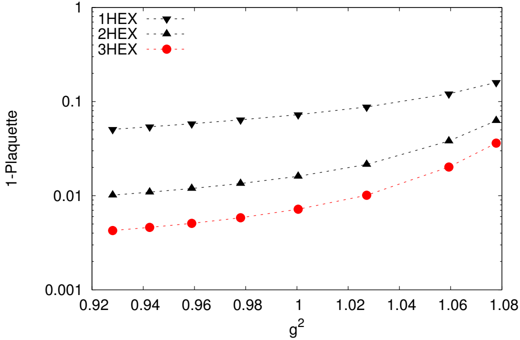
Unprecedented precision is required
$\Delta M_N / M_N = 0.14\% \rightarrow$ sub-permil precision is needed to get a high significance on ΔM_N

$m_u \neq m_d$ $\rightarrow$ 1+1+1+1 flavor lattice calculations are needed $\rightarrow$ algorithmic challenge
(Previous QCD calculations were typically 2+1 or 2+1+1 flavors)

Inclusion of QED: no mass gap
$\rightarrow$ power-like finite volume corrections expected
$\rightarrow$ long range photon field may cause large autocorrelations

HEX Smearing

Detailed test on pure gauge lattices with $L/r_0 = 3$
HEX parameters: $\rho_{\mathrm{HEX}} = (0.22, 0.15, 0.12)$



plaquette increases monotonically towards the continuum for 1,2 and 3 levels of HEX

Reflection positivity

A positive transfer matrix (Hermitian H) requires reflection positivity:

$$\langle (\Theta F) F \rangle \geq 0$$

where F is a function of fields at positive times, Θ is time reflection
Usual proof requires that the action

$$S = S_0 + S_- + S_+$$

where S_0, S_-, S_+ depend on $t <= 0, t = 0, t >= 0$ and $S_+ = \Theta S_-$

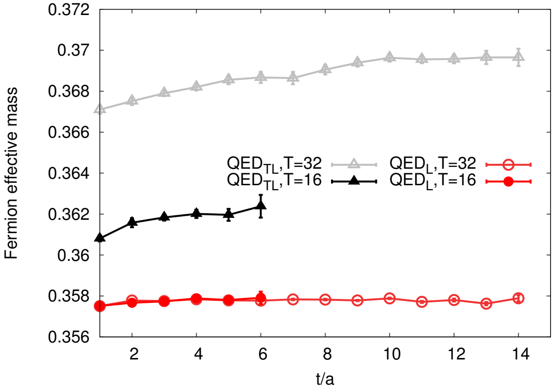
QED_{TL} condition can be implemented by including in the PI

$$\lim_{\xi \to 0} \exp \left[-\sum_\mu (a^4 \sum_x A_{\mu,x})^2 / \xi^2 \right] .$$

$\rightarrow \left(a^4 \sum_x A_{\mu,x}\right)^2$ term in S $\rightarrow$ spoils the proof (also num. evidence)

QED_L does not have this problem

Numerical tests of finite volume QED



Quenched QED simulations with fixed spatial size $L = 4$

QED_{TL}: no clear mass plateaux & mass increases with T

QED_L: clear plateaux, extracted mass T independent

Composite particles

In QCD charged hadrons are not point-like

previous results have to be extended

QED Ward identities $\rightarrow$ first two orders universal:

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

for scalars and spin half fermions

Form factors (e.g. charge radius) enter at $\mathcal{O}(\frac{\alpha}{L^3})$ level.

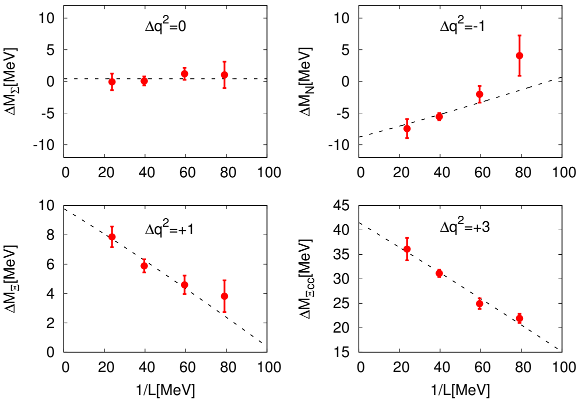
Strategy:

include analytic corrections for the two universal orders

fit coefficient of $1/L^3$

$1/L^3$ in many cases negligible, only significant for mesons

Finite V dependence of baryon masses



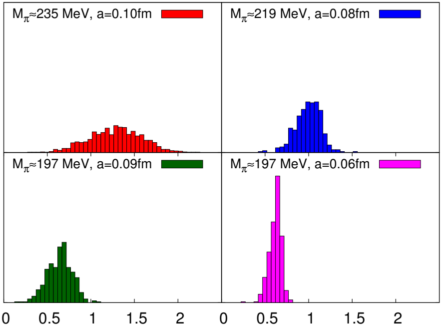
Σ splitting (identical charges) shows no volume dependence
V dependence of all baryons is well described by the universal part
$1/L^3$ order is insignificant for the volumes we use

Algorithmic challenges

Rational Hybrid Monte Carlo (RHMC) for all flavors

One flavor determinant not necessarily positive

Use $\sqrt{D^\dagger D}$ & inspect low eigenmodes to check correctness



Multi timescale, Hasenbusch trick & Omelyan integrator employed

Cost issues

Comparison to $N_f = 2 + 1$ physical mass calculations

- non-degenerate u,d quarks $\rightarrow$ factor 2
- typically two values of the electromagnetic coupling $\rightarrow$ factor 2
- physical m_u 40% smaller than average m_{ud} $\rightarrow$ $\approx 1.7\times$ slower inversions & $\approx 2.8\times$ larger volumes
- high precision determination of masses $\rightarrow$ factor 5 in statistics & factor 3 including analysis (many sources required)

Full analysis at physical point: $\approx 300\times$ the resources of 2+1 QCD $\rightarrow$ not yet realistic

Earlier spectroscopy + electroquenched results $\rightarrow$ with m_π down to 195 MeV one can reliably reach the physical point

Ensambles

strategy to tune to the physical point: 3+1 flavor simulations
pseudoscalar masses: $M_{\bar{q}q} = 410$ MeV and $M_{\bar{c}c} = 2980$ MeV
lattice spacings was determined by using $w_0 = 0.1755$ fm (fast)
for the final result a spectral quantity, M_Ω was used

series of $n_f = 1+1+1+1$ runs: QCDSF strategy
decreasing $m_{u/d}$ & increasing m_s by keeping the sum constant
small splitting in the mass of the up and down quarks
$\Longrightarrow$ 27 neutral ensembles with no QED interaction: e=0

turning on electromagnetism with $e = \sqrt{4\pi/137}, 0.71, 1$ and 1.41
significant change in the spectrum $\Rightarrow$ we compensate for it
additive mass: connected $M_{\bar{q}q}$ same as in the neutral ensemble
$\Longrightarrow$ 14 charged ensembles with various L and e
four ensembles for a large volume scan: L=2.4 ... 8.2 fm
five ensembles for a large electric charge scan: e=0 ... 1.41

Electric charge: signal/noise problem

symmetric operators under charge conjugation: depends on e^2
on a given gauge configuration (or on the level of the action):
no such symmetry, linear contribution in e
signal is proportional to e^2, whereas the noise is of $O(e)$

on electro-quenched configurations there is an elegant solution:
use a charge +e and a charge -e for the measurements
in the sum $O(e)$ parts drop out and only the quadratic remains
(the QED field generation has the +e versus -e symmetry)

for electro-unquenched configurations: no +e versus -e symmetry
dynamical configurations do feel the difference between up/down
due to their different charges they feel the QED field differently
small but important effect (we look for sub permil predictions)

Extracting hadron masses

fix the smeared photon and gluon fields to Coulomb gauge
quark fields are Gaussian smeared: smearing radius 0.3 fm
several hundred different source positions (reducing noise)
2-level multi-grid approach A. Frommer, K. Kahl, S. Krieg, B. Leder, M. Rottman, 1303.1377
variance reduction technique T. Blum, T. Izubuchi, E. Shintani, Phys. Rev. D88 094503 (2013)

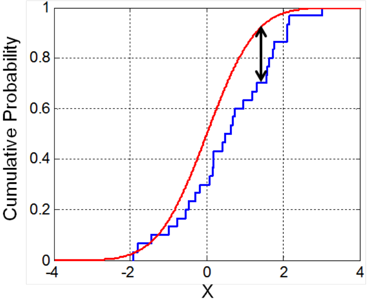
we jointly fit the isospin partners with the mass difference
(fit propagators separately and subtracting the fitted values)
stable correlation matrix: we only fit ten time slices
(large time slices usually do not provide any additional information)

which time slices (t_{min} and t_{max}) are the appropriate ones?
highly non-trivial choice (we are looking for sub-permil accuracy)

Kolmogorov-Smirnov analysis

select a good fit range: correlated χ^2/dof should be about one(?)
not really: χ^2/dof should follow instead the χ^2 distribution
probability that from t_{min} the χ^2/dof follow the distribution
(equivalently: goodnesses of the fits are uniformly distributed)

Kolmogorov-Smirnov: difference D (max. between the 2 distributions)



significance:

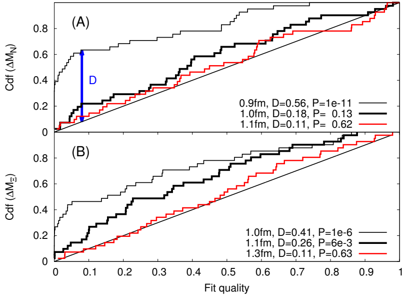
$$Q_{KS}(x) = 2\sum_j (-1)^{j-1} e^{-2j^2x^2}$$

with $Q_{KS}(0) = 1$ and $Q_{KS}(\infty) = 0$

Probablility(D>observed)
$=Q_{KS}([\sqrt{N} + 0.12 + 0.11/\sqrt{N}] \cdot D)$

Different fit intervals for the hadronic chanels

for each hadronic chanel: use the Kolmogorov-Smirnov test P>0.3



ΔM_N & ΔM_Ξ isospin mass differences with 41 ensembles
(with even more ensembles one can make it mass dependent)
the three t_{min} values give very different probabilities

ΔM_N: 1.1 fm; ΔM_Σ 1.1 fm; ΔM_Ξ 1.3 fm; ΔM_D 1.2 fm; $\Delta M_{\Xi cc}$: 1.2 fm

Reaching the physical point

similar strategy as in our spectrum paper S. Durr et al., Science 322 (2008) 1224

physical point is defined by: M_{π^+}=139.57 MeV, M_{K^+}=493.68 MeV, M_{K^0}=497.61 MeV, $M_{D^0} = 1864.9$ MeV
the electromagnetic coupling in the Thomson-limit $\alpha^{-1} = 137.036$
important input: kaon mass splitting ΔM_K^2=$M_{K^0}^2$-$M_{K^+}^2 = 3896$ MeV
overall scale is given by $M_\Omega = 1672.4$ MeV

for masses we used the values above; for α see earlier discussion

two methods: a. "mass-independent scale setting"; b. "ratio method"

a. traditional: $\beta \Rightarrow$ lattice spacing in the physical point
b. only mass ratios M_X/M_Ω extrapolated to the physical point

Determining the isospin splittings

two sources of isospin violation: electromagnetism & $m_u \neq m_d$

we work at larger than physical electromagnetic coupling values
renormalized coupling defined at hadronic scales

$\Rightarrow$ only linear term in α

$\delta m = m_d - m_u$ is very small $\Rightarrow$ linear term is also enough for δm

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

ΔM_K^2: QED-like L dependence: absorbed in $F_X(..., L, a)$
charged particle masses: corrected for universal finite-size effect
non-universal effects starting with $1/L^3$ are allowed in the QED part

alternative procedure: use ΔM_Σ (less precise) instead of ΔM_K^2
advantage: isospin partners with same charges, same L dependence
(carried out the complete analysis: yielded fully compatible results)

Choices for the extrapolating/interpolating functions

our standard approach Taylor expansion for the ΔM_X function

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

about 500 different choices for the functions (histogram method)
for $\alpha = 0$ and $m_u = m_d$ one obtains $\Delta M_X = 0$ (also for kaon)
$\Rightarrow F_X, G_X$ always start with constants (leading terms)

always use M_π^2, "a" in G_X, $1/L^3$ (non-universal) in F_X

lattice spacing dependence: $g^2 a$ (leading order) or a^2

optionally we add $M_{K^0}^2$, $M_{\pi^+}^4$ and M_{D^0} dependencies

many of the coefficients were consistent with zero

Separating QED and QCD effects

if α or $(m_u - m_d)$ vanishes QED or QCD parts disappear
separation: $\Delta M_X = \Delta_{\text{QED}} M_X + \Delta_{\text{QCD}} M_X$

it is sufficient to decompose the kaon mass squared difference

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

separation ambigous: depends on the choice of scheme for $m_u - m_d$
BMW electro-quenched analysis used connected $\Delta M^2 = M^2_{\bar{d}d} - M^2_{\bar{u}u}$
but connected mesons are not in the spectrum of the full theory

alternative separation: use Σ^+ and Σ^- baryons
they have the same charge squared and same spin
leading order: mass difference comes from strong isospin breaking
Gasser-Leutwyler correction with Cottingham formula 0.17(30) MeV
BMW-Coll.'s elecro-quenched result -0.08(12)(34) (large error)
using dynamical fields: $\Delta_{\text{QED}} M_\Sigma = 0.18(12)(6)$ MeV
all consistent with zero & much smaller than other uncertainties

Coleman-Glashow relation (1961)

suggestion: $\Delta_{\rm CG} = \Delta M_N - \Delta M_\Sigma + \Delta M_\Xi$ is close to zero

remember the quark compositions, in which it cancels indeed:
M(ddu)-M(uud)-M(sdd)+M(suu)+M(ssd)-M(ssu)=0

determine the leading order terms in the α and δm expansion

for α=0 a complete quark exchange symmetry
$\Delta_{\rm CG} \propto (m_s - m_d)(m_s - m_u)(m_d - m_u)$

for $\alpha > 0$ remains a $d \leftrightarrow s$ symmetry, thus $\Delta_{\rm CG} \propto \alpha(m_s - m_d)$

use $M_{sd}^2 = (M_{K+}^2 - M_{\pi+}^2)/2$, $\quad M_{du}^2 = \Delta_{QCD} M_K^2$ and $M_{su}^2 = M_{sd}^2 + M_{du}^2$

fit $\Delta_{\rm CG} = F_{\rm CG}(L,a) \cdot \alpha \cdot M_{sd}^2 + G_{\rm CG}(a) \cdot M_{sd}^2 M_{su}^2 M_{du}^2$

the Coleman-Glashow relation is satisfied to high accuracy

$$\Delta_{\rm CG} = 0.00(11)(06)\ \text{MeV}$$

Chosing the fitting functions: Kullback–Leibler

we have several fit functions with different number of parameters

$\Gamma_1, \dots, \Gamma_n$ measurements from (unknown) PDF $g^{(1)}(\Gamma)$
$f^{(1)}(\Gamma|\theta)$ is one model with $\theta_1, \dots, \theta_p$ parameters

Kullback–Leibler divergence: difference of f from g (always $\geq$0)

$$I(g, f(\theta)) = \int \mathrm{d}\Gamma \; g(\Gamma) \log[g(\Gamma)/f(\Gamma|\theta)]$$

joint PDF: $g(\Gamma) = \prod_{k=1}^{n} g^{(1)}(\Gamma_k)$ (same for f)

consider each model with $w_m \propto$ probability it reproduces the data

$$w_m = \frac{\exp\left[-I(g, f_m(\theta_m))\right]}{\sum_{m'} \exp\left[-I(g, f_{m'}(\theta_{m'}))\right]}$$

determine $I(g, f(\theta))$ (on the right hand side g·log(g) is constant)

Akaike's information criterion

first find $\hat{\theta}$ which maximizes $J_m(\Gamma) = \int \mathrm{d}\Gamma\ g(\Gamma) \log[f_m(\Gamma|\theta)]$
then determine J_m (as we mentioned the PDF g is unknown)

if a. $n \to \infty$ b. f is close to g
$J_m(\Gamma)$ can be estimated by -$\frac{1}{2} AIC_m(\Gamma) = \log[f(\Gamma|\hat{\theta}_{m,\Gamma})] - p_m$
(derivation: complicated; can not be easily found in the literature)

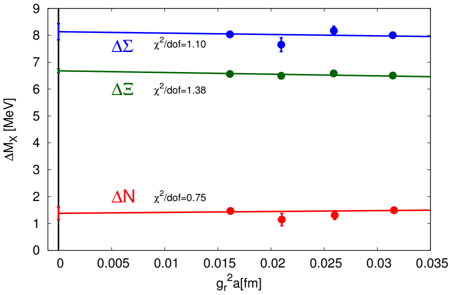
use the weights obtained by determining $J_m(\Gamma)$ values
normally distributed errors: $\mathrm{AIC}_m(\Gamma) = \chi^2_m + 2p_m$
AIC weight prefers models with lower χ^2 values
but punishes models with too many fit parameters

von Neumann used to say: with four parameters I can fit an elephant, and with five I can make him wiggle his trunk (E. Fermi 1953)

Getting the final results

extra- and interpolations to the physical point
a. mass-independent or ratio method; b. form for ΔM_X
c. two different fitting ranges d. $(8\tau)^{-1/2} = 280/525$ MeV for α

$\mathcal{O}(500)$ fits, for which we use AIC/goodness/no weights



essentially no lattice spacing dependence (also small for M_π)

Systematic uncertainties/blind analysis

various fits go into BMW Collaboration's hystogram method
its mean: central value with the central 68%: systematic error
use AIC/goodness/no: same result within 0.2σ (except Ξ_{cc}: 0.7σ)
2000 bootstrap samples: statistical uncertainty

ΔM_X has tiny errors, it is down on the 0.1 permil level
many of them are known $\Longrightarrow$ possible bias $\Longrightarrow$ blind analysis

medical research: double-blind randomized clinical trial (Hill, 1948)
both clinicians and patients are not aware of the treatement
physics: e/m of the electron with angle shift (Dunnington 1933)

we extracted M_X & multiplied by a random number between 0.7–1.3
the person analysing the data did not know the value $\Longrightarrow$
reintroduce the random number $\Longrightarrow$ physical result (agreement)